(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
8 November 2001 (08.11.2001)

PCT

(10) International Publication Number
WO 01/83717 A2

(51) International Patent Classification[7]: C12N 9/00

(21) International Application Number: PCT/CA01/00607

(22) International Filing Date: 2 May 2001 (02.05.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/201,841 3 May 2000 (03.05.2000) US

(71) Applicant *(for all designated States except US)*: **GLYCODESIGN INC.** [CA/CA]; 480 University Avenue, Suite 400, Toronto, Ontario M5G 1V2 (CA).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **RAO, Mohan** [IN/CA]; 95 Thorncliffe Park Drive, Apartment 3409, Toronto, Ontario M4H 1L7 (CA). **TVAROSKA, Igor** [SK/CA]; 65 High Park Avenue, Apartment 2201, Toronto, Ontario M6P 2R7 (CA).

(74) Agents: **VAN ZANT, Joan M.** et al.; Swabey Ogilvy Renault, Suite 1600, 1981 McGill College Avenue, Montreal, Québec H3A 2Y3 (CA).

(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW.

(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
— *without international search report and to be republished upon receipt of that report*

[Continued on next page]

(54) Title: DESIGNING MODULATORS FOR GALACTOSYLTRANSFERASES

(57) Abstract: The invention relates to structures and models of ligand binding domains of galactosyltransferases, and the ligand binding domains with ligands. The structural coordinates that define the structures and any ligands bound to the structures enable the determination of homologues, the structures of polypeptides with unknown structure, and the identification of modulators of the galactosyltransferases. The invention also relates to structures and models of nucleotide-sugar donors for the galactosyltransferases, and the design of modulators for the galactosyltransferases based on the properties of these structures and models.

WO 01/83717 A2

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

TITLE: Designing Modulators for Galactosyltransferases

FIELD OF THE INVENTION

The invention relates to structures and models of ligand binding domains of galactosyltransferases, and the ligand binding domains with ligands. The structural coordinates that define the structures and any ligands bound to the structures enable the determination of homologues, the structures of polypeptides with unknown structure, and the identification of modulators of the galactosyltransferases. The invention also relates to structures and models of nucleotide-sugar donors for the galactosyltransferases, and the design of modulators for the galactosyltransferases based on the properties of these structures and models.

BACKGROUND OF THE INVENTION

Carbohydrate groups of glycoproteins are involved in various signaling and molecular recognition processes leading to important biological functions (1) and diseases (2). The processing and synthesis of a large number of both *N*- and *O*- linked carbohydrate chains involve the sequential and coordinated action of many different glycosyltransferases. Glycosyltransferases catalyze the transfer of monosaccharide from nucleotide sugars to a specific hydroxyl of various saccharide acceptors that leads to the formation of a new glycosidic linkage. There is at least one distinct glycosyltransferase for every type of glycosidic linkage.

Galactosyltransferases are a class of enzymes that utilize uridine-5'-diphosphogalactose (UDP-Gal) as the donor. Recently, a retaining galactosyltransferase, α-1,3-galactosyltransferase (α-1-3GalT; E.C.2.4.1.151) (4) has attracted much attention due to a problem of organ rejection in xenotransplantation. This enzyme is responsible for the formation of terminal α-Gal sequences in Galα1-3 Galβ1- GlcNAcα1-R. Oligosaccharide structures with a terminal Galα1-3Galβ sequence (α-galactosyl epitopes) are xenoactive antigens (5) and are considered to be the major cause of hyperacute rejections in xenotransplantation. α-1,3-Galactosyltransferase is absent in humans and, conversely, large quantities of natural anti-α-1,3-Gal antibodies exist in the human body which react with the α-Gal epitope, thus providing a barrier to xenotransplant. The appearance of aberrant α-1,3-GalT in human cells is assumed to be responsible for some forms of anti-immune diseases (6).

Galactosyltransferases share a common topology with type II membrane proteins. Type II membrane proteins generally have a large N-terminal catalytic domain, a short stem region and a hydrophobic rich transmembrane domain (3). Although, various groups have performed a host of biochemical studies on this enzyme to understand structure-function relationships, the actual binding and catalytic mechanism of α-1,3-GalT is poorly understood. For an understanding of these important aspects in atomic detail it is essential to have a three-dimensional structure of α-1,3-GalT and structural information about the binding of UDP-Gal and oligosaccharide acceptor in the active site of α-1,3-GalT. Unfortunately, no crystal structure is available on α-1,3-GalT in native or complexed form.

SUMMARY OF THE INVENTION

The present inventors have produced a homology model for galactosyltransferases, and complexes of the enzymes with ligands including UDP and UDP-Gal. The homology model was developed by means of molecular modeling using the SpsA glycosyltransferase structure. In particular, a protein-ligand docking approach was used to model α-1,3-GalT complexed with UDP and UDP-Gal. In the predicted model complex, the diphosphate interacts with a DVD motif (Asp-225, Val-226 and Asp-227) of α-1-3GalT through a Mn^{2+} cation. The uridine part of the UDP binds into the cavity that consists of Phe-134, Tyr-139, Ile-140, Val-136, Arg-194, Arg-202, Lys-209, Asp-

173, His-218, and Thr-137, in a "canonical conformation". Structural features of the α-1,3-GalT model were compared with available structural data on this class of enzymes and revealed similarities in the UDP binding pocket.

The invention provides a model or secondary, tertiary, and/or quanternary structure of a ligand binding domain of a galactosyltransferase. Binding domains are of significant utility in drug discovery. The association of natural ligands and substrates with the binding domains of galactosyltransferases is the basis of biological mechanisms. The associations may occur with all or any parts of a binding domain. An understanding of these associations will lead to the design and optimization of drugs having more favorable associations with their target enzyme and thus provide improved biological effects. Therefore, information about the shape and structure of galactosyltransferases and their ligand-binding domains is invaluable in designing potential modulators of galactosyltransferases for use in treating diseases and conditions associated with or modulated by the galactosyltransferases.

Ligand binding domains include one or more of the binding domains for a disphosphate group of a sugar nucleotide donor, a nucleotide of a sugar nucleotide donor, a nitrogeneous heterocyclic base (preferably a pyrimidine base, more preferably uracil) of a sugar nucleotide donor, a sugar of the nucleotide of a sugar nucleotide donor, a selected sugar of a sugar nucleotide donor that is transferred to an acceptor, and/or an acceptor. The structure of a ligand binding domain may be defined by selected binding sites in the domain.

Thus, broadly stated the present invention provides a model or a secondary or three dimensional structure of a ligand binding domain of a galactosyltransferase comprising one or more of the amino acid residues shown in Table 1 or Figure 2, 3, 4, or 6.

The invention also relates to a model or a secondary or three dimensional structure of a ligand binding domain of a galactosyltransferase defined by the structural coordinates of one or more of the atomic interactions or contacts of Table 1. Each of the atomic interactions is defined in Table 1 by an atomic contact (more preferably a specific atom where indicated) on the sugar nucleotide donor and an atomic contact (more preferably a specific atom where indicated) on the galactosyltransferase.

In accordance with an aspect of the invention, there is also provided a model of a ligand binding domain designed in accordance with a method of the invention and comprising hydrogen binding partners for the amide hydrogen, carbonyl oxygen in position 4, and the carbonyl oxygen of uracil.

The invention also provides a model of a ligand binding domain that binds the uridine portion of UDP and comprises two or more of Phe-134, Tyr-139, Ile-140, Val-136, Arg-194, Arg-202, Lys-209 (numbered as ATOM 204 in Table 8), Asp-173 (numbered as ATOM 169 in Table 8), His-218 (numbered as ATOM 213 in Table 8), and Thr-137 (numbered as ATOM 132 in Table 8). The invention also provides a model of a ligand binding domain that interacts with a pyrophosphate portion of UDP comprising Asp-225, Val-226, and Asp-227.

The invention provides a model or secondary, tertiary and/or quanternary structure of a galactosyltransferase.

The invention contemplates a model or secondary, tertiary and/or quanternary structure of a galactosyltransferase in association with a ligand or substrate.

The structures and models of the invention provide information about the atomic contacts involved in the interaction between the enzyme and a known ligand which can be used to screen for unknown ligands. Therefore the present invention provides a method of screening for a ligand capable of binding a galactosyltransferase ligand

binding domain, comprising the use of a secondary or three-dimensional structure or a model of the invention. For example, the method may comprise the step of contacting a ligand binding domain with a test compound, and determining if the test compound binds to the ligand.

A method of the invention may identify a ligand which can modulate the biological activity of a galactosyltransferase. Such a ligand is referred to herein as a "modulator". In an embodiment, the present invention contemplates a method of identifying a modulator of a galactosyltransferase or a ligand binding domain or binding site thereof, comprising the step of using the structural coordinates of a galactosyltransferase or a ligand binding domain or binding site thereof, or a model of the invention to computationally evaluate a test compound for its ability to associate with the galactosyltransferase or ligand binding domain or binding site thereof. Use of the structural coordinates of a galactosyltransferase structure, ligand binding domain, or binding site thereof, of the invention to identify a ligand or modulator is also provided.

A structure or model of the invention may be used to design, evaluate, and identify ligands of galactosyltransferases other than ligands that associate with a galactosyltransferase. The ligands may be based on the shape and structure of a galactosyltransferase, or a ligand binding domain or atomic interactions, or atomic contacts thereof. Therefore, ligands, in particular modulators, may be derived from ligand binding domains or analogues or parts thereof.

The present invention also contemplates a ligand identified by a method of the invention. A ligand may be a competitive or non-competitive inhibitor of a galactosyltransferase. Preferably, the ligand is capable of modulating the activity of a galactosyltransferase enzyme. Thus the methods of the invention permit the identification early in the drug development cycle of compounds that have advantageous properties.

In an embodiment of the invention, a method is provided for identifying a potential modulator of a galactosyltransferase by determining binding interactions between a test compound and atomic contacts of a binding domain of a galactosyltransferase defined in accordance with the invention comprising:

(a) generating the atomic contacts on a computer screen;

(b) generating test compounds with their spatial structure on the computer screen; and

(c) determining whether the compounds associate or interact with the atomic contacts defining the galactosyltransferase;

(d) identifying test compounds that are potential modulators by their ability to enter into a selected number of atomic contacts.

Another aspect of the invention provides methods for identifying a potential modulator of a galactosyltransferase function by docking a computer representation of a test compound with a computer representation of a structure of a galactosyltransferase or a ligand binding domain thereof that is defined as described herein. In an embodiment the method comprises the following steps:

(a) docking a computer representation of a compound from a computer data base with a computer representation of atomic interactions or contacts of a ligand binding domain of a galactosyltransferase to obtain a complex;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying test compounds that best fit the atomic interactions or contacts as potential modulators of the galactosyltransferase.

In another embodiment the method comprises the following steps:

(a) modifying a computer representation of a test compound complexed with a ligand binding domain of a galactosyltransferase by deleting or adding a chemical group or groups;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying a test compound that best fits the ligand binding domain as a potential modulator of a galactosyltransferase.

In still another embodiment the method comprises the following steps:

(a) selecting a computer representation of a test compound complexed with atomic contacts of a binding domain of a galactosyltransferase; and

(b) searching for molecules in a data base that are similar to the test compound using a searching computer program, or replacing portions of the test compound with similar chemical structures from a data base using a compound building computer program.

The ligands or compounds identified according to the methods of the invention preferably have structures such that they are able to enter into an association with a ligand binding domain. Selected ligands or compounds may be characterized by their suitability for binding to particular binding domains. A ligand binding domain or binding site may be regarded as a type of negative template with which the compounds correlate as positives in the manner described herein and thus the compounds are unambiguously defined. Therefore, it is possible to describe the structure of a compound suitable as a modulator of a galactosyltransferase by accurately defining the atomic interactions to which the compound binds to a ligand binding domain and deriving the structure of the compound from the spacial structure of the target.

The invention contemplates a method for the design of ligands, in particular modulators, for galactosyltransferases based on the three dimensional structure of a sugar nucleotide donor (or part thereof) defined in relation to its spatial association with the three dimensional structure of the galactosyltransferase or a ligand binding domain thereof. Generally, a method is provided for designing potential inhibitors of a galactosyltransferase comprising the step of using the structural coordinates of a sugar nucleotide donor or part thereof, defined in relation to its spatial association with a three dimensional structure or model of a galactosyltransferase or a ligand binding domain thereof, to generate a compound for associating with a ligand binding domain of the galactosyltransferase. The following steps are employed in a particular method of the invention: (a) generating a computer representation of a sugar nucleotide donor, or part thereof, defined in relation to its spatial association with the three dimensional structure of a galactosyltransferase or a ligand binding domain thereof; (b) searching for molecules in a data base that are similar to the defined sugar nucleotide donor, or part thereof, using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

Therefore the invention further contemplates classes of ligands, in particular modulators, of a galactosyltransferase based on the three-dimensional structure of a sugar nucleotide donor, or part thereof, defined in relation to the sugar nucleotide donor's spatial association with a three dimensional structure of a galactosyltranferase.

It will be appreciated that a ligand or modulator of a galactosyltransferase may be identified by generating an actual secondary or three-dimensional model of a ligand binding domain or binding site, synthesizing a compound, and examining the components to find whether the required interaction occurs.

Modulators which are capable of modulating the activity of galactosyltransferases have therapeutic and prophylactic potential. Therefore, the methods of the invention for identifying modulators may comprise one or more of the following additional steps:

(a) testing whether the ligand is a modulator of the activity of a galactosyltransferase, preferably testing the activity of the modulator in cellular assays and animal model assays;

(b) modifying the modulator;

(c) optionally rerunning steps (a) or (b); and

(d) preparing a pharmaceutical composition comprising the modulator.

Steps (a), (b) (c) and (d) may be carried out in any order, at different points in time, and they need not be sequential.

There is also provided a pharmaceutical composition comprising a modulator, and a method of treating and/or preventing disease comprising the step of administering a modulator or pharmaceutical composition comprising a modulator to a mammalian patient.

In an aspect, the invention contemplates a method of treating a disease associated with a galactosyltransferase with inappropriate activity in a cellular organism, comprising:

(a) administering a modulator identified using the methods of the invention in an acceptable pharmaceutical preparation; and

(b) activating or inhibiting a galactosyltransferase to treat the disease.

The invention provides for the use of a modulator identified by the methods of the invention in the preparation of a medicament to treat a disease associated with a galactosyltransferase with inappropriate activity in a cellular organism. Use of the structural coordinates of a galactosyltransferase structure of the invention to manufacture a medicament is also provided.

Another aspect of the invention provides machine readable media encoded with data representing a model of the invention or the coordinates of a structure of a galactosyltransferase or ligand binding domain or binding site thereof as defined herein, or the three dimensional structure of a sugar nucleotide donor defined in relation to its spatial association with a three dimensional structure of a galactosyltransferase as defined herein. The invention also provides computerized representations of a model of the invention or the secondary or three-dimensional structures of the invention , including any electronic, magnetic, or electromagnetic storage forms of the data needed to define the structures such that the data will be computer readable for purposes of display and/or manipulation. The invention further provides a computer programmed with a homology model of a ligand binding domain of a galactosyltransferase. The invention still further contemplates the use of a homology model of the invention as input to a computer programmed for drug design and/or database searching and/or molecular graphic imaging in order to identify new ligands for galactosyltransferases.

These and other aspects of the present invention will become evident upon reference to the following detailed description and attached drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

The invention will now be described in relation to the drawings in which:

Figure 1. Sequence alignment between SpsA and bovine α-1,3-GalT.

Figure 2. A superposition of the SpsA structure and the α-1,3-GalT model. The active site residues of SpsA and the corresponding residues of α-1,3-GalT are shown as tubes. SpsA is shown in magenta and α-1,3-GalT is in blue. The side-chains of the α-1,3-GalT model are labeled. The active site modeled metal ion is shown as a red sphere.

Figure 3. The low-energy computed docking modes of UDP to the α-1,3-GalT. About 60 low energy binding modes of UDP are shown in colored lines. The lowest energy binding mode is shown in thick tube. The critical amino acid residues are shown and labeled. All the low energy binders assume similar binding orientation.

Figure 4. Possible docking modes of UDP-Gal to the α1,3-GalT. The lowest-energy docking mode is shown as thick tube and some of the low energy binding modes are shown as thin lines.

Figure 5. The predicted complex of α-1-3GalT and the inhibitor. Two top ranking docking modes are shown and in both, the inhibitor occupies the acceptor and pyrophosphate binding regions of the α-1,3-GalT. The lowest energy-binding mode is shown in thick tube.

Figure 6 shows the overall view of a docking model of bovine alpha 1,3 galT-UDP complex. GalT is shown in colored ribbon. The UDP is shown in think tubes. The amino acid residues that interact with UDP are shown in tubes and the modeled Mn^{2+} is shown in a sphere. The conserved DVD motif interaction with a metal can be seen.

Figure 7 shows an overall representation of the UDP-Gal complex.

Figure 8 shows computed low energy binding modes of UDP-Gal.

Figure 9 shows lowest energy binding modes of LacNAc-β-Ome to α-1,3-GalT.

DESCRIPTION OF THE TABLES

Table 1 – Atomic interactions between a galactosyltransferase and UDP.

Table 2 – Characterization of the top five binding modes of UDP to α-1,3-galactosyltransfease.

Table 3 - Predicted secondary structures for the α-1,3-GalT sequence that was used for generating a homology model of α-1,3-GalT.

Table 4 – Structural coordinates of a galactosyltransferase

Table 5 - Structural coordinates of UDP.

Table 6 – Structural coordinates of UDP-Gal.

Table 7 – Structural coordinates of uracil, ribose, and pyrophosphate of UDP.

Table 8 – Structural coordinates of a galactosyltransferases.

In Table 4, from the left, the second column identifies the atom number; the third identifies the atom type; the fourth identifies the amino acid type; the fifth identifies the residue number; the sixth identifies the x coordinates; the seventh identifies the y coordinates; and the eighth identifies the z coordinates.

DETAILED DESCRIPTION OF PREFERRED EMBODIMENTS

Definitions:

Unless otherwise indicated, all terms used herein have the same meaning as they would to one skilled in the art of the present invention. Practitioners are particularly directed to Current Protocols in Molecular Biology

(Ansubel) for definitions and terms of the art. Abbreviations for amino acid residues are the standard 3-letter and/or 1-letter codes used in the art to refer to one of the 20 common L-amino acids.

The term "associate", "association" or "associating" refers to a condition of proximity between a ligand, chemical entity or compound or portions or fragments thereof, and a galactosyltransferase, or portions or fragments thereof (e.g. ligand binding domain). The association may be non-covalent i.e. where the juxtaposition is energetically favored by for example, hydrogen-bonding, van der Waals, or electrostatic or hydrophobic interactions, or it may be covalent.

The term "galactosyltransferase" refers to an enzyme that catalyzes the transfer of a single monosaccharide unit i.e. galactose, from a donor to the hydroxyl group of an acceptor saccharide. The acceptor can be either a free saccharide, glycoprotein, glycolipid, or polysaccharide. The donor can be a sugar nucleotide, preferably UDP-Gal. Galactosyltransferases show a precise specificity for both the sugar acceptor and donor and generally require the presence of a metal cofactor.

Galactosyltransferases are derivable from a variety of sources, including viruses, bacteria, fungi, plants, and animals. In a preferred embodiment the galactosytransferases are derivable from an animal, preferably a mammal including but not limited to bovine, ovine, porcine, murine equine, most preferably a human. The enzyme may be from any source, whether natural, synthetic, semi-synthetic, or recombinant. Preferably the galactosyltransferase is a α1-3 galactosyltransferase, preferably derivable from bovine.

A galactosyltransferase or part thereof in the present invention may be a wild type enzyme, or part thereof, or a mutant, variant or homologue of such an enzyme.

The term "wild type" refers to a polypeptide having a primary amino acid sequence which is identical with the native enzyme (for example, the mammalian enzyme).

The term "mutant" refers to a polypeptide having a primary amino acid sequence which differs from the wild type sequence by one or more amino acid additions, substitutions or deletions. Preferably, the mutant has at least 90% sequence identity with the wild type sequence. Preferably, the mutant has 20 mutations or less over the whole wild-type sequence. More preferably the mutant has 10 mutations or less, most preferably 5 mutations or less over the whole wild-type sequence. A mutant may or may not be functional.

The term "variant" refers to a naturally occurring polypeptide which differs from a wild-type sequence. A variant may be found within the same species (i.e. if there is more than one isoform of the enzyme) or may be found within a different species. Preferably the variant has at least 90% sequence identity with the wild type sequence. Preferably, the variant has 20 mutations or less over the whole wild-type sequence. More preferably, the variant has 10 mutations or less, most preferably 5 mutations or less over the whole wild-type sequence.

The term "part" indicates that the polypeptide comprises a fraction of the wild-type amino acid sequence. It may comprise one or more large contiguous sections of sequence or a plurality of small sections. The "part" may comprise a ligand binding domain as described herein. The polypeptide may also comprise other elements of sequence, for example, it may be a fusion protein with another protein. Preferably the polypeptide comprises at least 50%, more preferably at least 65%, most preferably at least 80% of the wild-type sequence.

The term "homologue" means a polypeptide having a degree of homology with the wild-type amino acid sequence. The term "homology" can be equated with "identity".

In the present context, a homologous sequence is taken to include an amino acid sequence which may be at least 75, 85 or 90% identical, preferably at least 95 or 98% identical to the wild-type sequence. Typically, the

homologues will comprise the same sites (for example ligand binding domain) as the subject amino acid sequence. Although homology can also be considered in terms of similarity (i.e. amino acid residues having similar chemical properties/functions), in the context of the present invention it is preferred to express homology in terms of sequence identity.

Homology comparisons can be conducted by eye, or more usually, with the aid of readily available sequence comparison programs. These commercially available computer programs can calculate % homology between two or more sequences (e.g. Wilbur, W.J. and Lipman, D. J. Proc. Natl. Acad. Sci. USA (1983), 80:726-730).

The term "function" refers to the ability of a modulator to enhance or inhibit the association between a galactosyltransferase and a compound, or the activity of the galactosyltransferase.

"Ligand binding domain" refers to a region of a molecule or molecular complex that as a result of its shape, favourably associates with a ligand or a part thereof. For example, it may be a region of a galactoysltransferase that is responsible for binding a substrate or known modulator.

The term "ligand binding domain" includes homologues of a ligand binding domain or portions thereof. As used herein, the term "homologue" in reference to a ligand binding domain refers to a ligand binding domain or a portion thereof which may have deletions, insertions or substitutions of amino acid residues as long as the binding specificity of the molecule is retained. In this regard, deliberate amino acid substitutions may be made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity, and/or the amphipathic nature of the residues as long as the binding specificity of the ligand binding domain is retained.

As used herein, the term "portion thereof" means the structural coordinates corresponding to a sufficient number of amino acid residues of a galactosyltransferase ligand binding domain (or homologues thereof) that are capable of associating with or interacting with a test compound that binds to the ligand binding domain. This term includes galactosyltransferase ligand binding domain amino acid residues having amino acid residues from about 4Å to about 5Å of a bound compound or fragment thereof. Thus, for example, the structural coordinates provided in the structure may contain a subset of the amino acid residues in the ligand binding domain which may be useful in the modelling and design of compounds that bind to the ligand binding domain.

A ligand binding domain may be defined by its association with a ligand. With reference to the structures and models of the invention, residues in the ligand binding domain may be defined by their spatial proximity to a ligand. For example, such may be defined by their proximity to a substrate or modulator.

A ligand binding domain of the invention may comprise a DVD motif comprising one or more of Asp-225, Val-226, and Asp-227. A ligand binding domain may comprise one or more of Phe-134, Tyr-139, Ile-140, Val-136, Arg-194, Arg-202, Lys-209 (numbered as ATOM 204 in Table 8), Asp-173 (numbered as ATOM 169 in Table 8), His-218 (numbered as ATOM 213 in Table 8), and Thr-137 (numbered as ATOM 132 in Table 8) that binds uridine.

"Ligand" refers to a compound or entity that associates with a ligand binding domain, including substrates or analogues or parts thereof. A ligand may be designed rationally using a model according to the invention. A ligand may be a modulator.

"Modulator" refers to a molecule which changes or alters the biological activity of a galactosyltransferase. A modulator may increase or decrease galactosyltransferase activity, or change its characteristics, or functional or immunological properties. It may be an inhibitor that decreases the biological or immunological activity of the protein. A modulator may include but is not limited to peptides, members of random peptide libraries and

combinatorial chemistry-derived molecular libraries, phosphopeptides (including members of random or partially degenerate, directed phosphopeptide libraries), antibodies, carbohydrates, monosaccharides, oligosaccharides, polysaccharides, glycolipids, saponins, heterocyclic compounds, nucleosides or nucleotides or parts thereof, and small organic or inorganic molecules. A modulator may be an endogenous physiological compound or it may be a natural or synthetic compound. The term "modulator" also refers to a chemically modified ligand or compound, and includes isomers and racemic forms.

The term "structural coordinates" as used refers to a set of values that define the position of one or more amino acid residues with reference to a system of axes. A data set of structural coordinates defines the three dimensional structure of a molecule or molecules. Structural coordinates can be slightly modified and still render nearly identical three dimensional structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 2 Å, preferably less than 0.5 Å, more preferably less than 0.3 Å, may be viewed by a person of ordinary skill in the art as identical.

Variations in structural coordinates may be generated because of mathematical manipulations of the structural coordinates of a galactosyltransferase described herein. For example, the structural coordinates of Table 4 or 8 may be manipulated by crystallographic permutations of the structural coordinates, fractionalization of the structural coordinates, integer additions or substractions to sets of the structural coordinates, inversion of the structural coordinates or any combination of the above.

Variations in structure due to mutations, additions, substitutions, and/or deletions of the amino acids, or other changes in any of the components that make up a structure of the invention may also account for modifications in structural coordinates. If such modifications are within an acceptable standard error as compared to the original structural coordinates, the resulting structure may be the same. Therefore, a ligand that associates with or binds to a ligand binding domain of a galactosyltransferase would also be expected to associate with or bind to another ligand binding domain whose structural coordinates defined a shape that fell within the acceptable error. Such modified structures of a ligand binding domain are also within the scope of the invention.

Various computational analyses may be used to determine whether a ligand or the ligand binding domain thereof is sufficiently similar to all or parts of a ligand or ligand binding domain of the invention. Such analyses may be carried out using conventional software applications and methods as described herein.

The term "modeling" includes the quantitative and qualitative analysis of molecular structure and/or function based on atomic structural information and interaction models. The term includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry, and other structure-based constraint models. Preferably modeling is performed using a computer and may be optimized using known methods. This is called modeling optimization.

The term "substrate" refers to molecules that associate with a galactosyltransferase as it catalyzes the transfer of a selected sugar from a nucleotide sugar donor to an acceptor that leads to the formation of a new glycosidic linkage. A substrate includes a sugar nucleotide donor and acceptor and parts thereof.

A "sugar nucleotide donor" refers to a nucleotide coupled to a selected sugar that is transferred by a galactosyltransferase to an acceptor. The selected sugar may be a monosaccharide or disaccharide, preferably a monosaccharide. A suitable selected sugar includes galactose. The galatose may be modified for example, the hydroxyls may be blocked with acetonide, acylated, or alkylated or substituted with other groups such as halogen.

The nucleotide is preferably UDP. The heterocyclic amine base in the nucleotide may be modified. For example, when the base is uridine it may be modified at the C-5 or C-6 position with groups including but not limited to alkyl, aryl, gallic acid, and with electron donating and electron withdrawing groups. The sugar in the nucleotide (e.g. ribose) may be modified at the 2' or 3' position with groups including but not limited to alkyl, aryl, gallic acid, and with electron donating and electron withdrawing groups.

An "acceptor" refers to the part of a carbohydrate structure (e.g. glycoprotein, glycolipid) where the selected sugar of a sugar nucleotide donor is transferred by the galactosyltransferase.

The term "alkyl", alone or in combination, refers to a branched or linear hydrocarbon radical, typically containing from 1 through 20 carbon atoms, preferably 1 through 10 carbon atoms, more preferably 1 to 6 carbon atoms. Typical alkyl groups include but are not limited to methyl, ethyl, 1-propyl, 2-propyl, 1-butyl, 2-butyl, tert-butyl, pentyl, hexyl, heptyl, octyl, nonyl, decyl, and the like.

The term "alkenyl", alone or in combination, refers to an unsaturated branched or linear group typically having from 2 to 20 carbon atoms and at least one double bond. Examples of such groups include but are not limited to ethenyl, 1-propenyl, 2-propenyl, 1-butenyl, 1,3-butadienyl, 1-hexenyl, 2-hexenyl, 1-pentenyl, 2-pentenyl, and the like.

The term "alkynyl", alone or in combination, refers to an unsaturated branched or linear group having 2 to 20 carbon atoms and at least one triple bond. Examples of such groups include but are not limited to ethynyl, 1-propynyl, 2-propynyl, 1-butynyl, 2-butynyl, 1-pentynyl, and the like.

The term "cycloalkyl" refers to cyclic hydrocarbon groups and includes but is not limited to cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, cycloheptyl, and cyclooctyl.

The term "aryl", alone or in combination, refers to a monocyclic or polycyclic group, preferably a monocyclic or bicyclic group. An aryl group may optionally be substituted as described herein. Examples of aryl groups and substituted aryl groups are phenyl, benzyl, p-nitrobenzyl, p-methoxybenzyl, biphenyl, and naphthyl.

The term "alkoxy" alone or in combination, refers to an alkyl or cycloalkyl linked to the parent molecular moiety through an oxygen atom. The term "aryloxy" refers to an aryl linked to the parent molecular moiety through an oxygen atom. Examples of alkoxy groups are methoxy, ethoxy, propoxy, vinyloxy, allyloxy, butoxy, pentoxy, hexoxy, cyclopentoxy, and cyclohexoxy. Examples of aryloxy groups are phenyloxy, O-benzyl i.e. benzyloxy, O-p-nitrobenzyl and O-p-methyl-benzyl, 4-nitrophenyloxy, 4-chlorophenyloxy, and the like.

The term "halo" or "halogen", alone or in combination, means fluoro, chloro, bromo, or iodo.

The term "amino", alone or in combination, refers to a chemical functional group where a nitrogen atom (N) is bonded to three substituents being any combination of hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, or aryl with the general chemical formula $-NR_{14}R_{16}$ where R_{14} and R_{16} can be any combination of hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, or aryl. Optionally one substituent on the nitrogen atom can be a hydroxyl group (-OH) to give an amine known as a hydroxylamine. Examples of amino groups are amino ($-NH_2$), methylamine, ethylamine, dimethylamine, 2-propylamine, butylamine, isobutylamine, cyclopropylamine, benzylamine, allylamine, hydroxylamine, cyclohexylamino ($-NHCH(CH_2)_5$), piperidine ($-N(CH_2)_5$) and benzylamino ($-NHCH_2C_6H_5$).

The term "thioalkyl", alone or in combination, refers to a chemical functional group where a sulfur atom (S) is bonded to an alkyl. Examples of thioalkyl groups are thiomethyl, thioethyl, and thiopropyl.

The term "thioaryl", alone or in combination, refers to a chemical functional group where a sulfur atom (S) is bonded to an aryl group with the general chemical formula $-SR_{16}$ where R_{16} is an aryl group which may be

substituted. Examples of thioaryl groups and substituted thioaryl groups are thiophenyl, para-chlorothiophenyl, thiobenzyl, 4-methoxy-thiophenyl, 4-nitro-thiophenyl, and para-nitrothiobenzyl.

Heterocyclic rings are molecular rings where one or more carbon atoms have been replaced by hetero atoms (atoms not being carbon) such as for example, oxygen (O), nitrogen (N) or sulfur (S), or combinations thereof. Examples of heterocyclic rings include ethylene oxide, tetrahydrofuran, thiophene, piperidine (piperidinyl group), pyridine (pyridinyl group), and caprolactam. A carbocyclic or heterocyclic group may be optionally substituted at carbon or nitrogen atoms with for example, alkyl, phenyl, benzyl or thienyl, or a carbon atom in the heterocyclic group together with an oxygen atom may form a carbonyl group, or a heterocyclic group may be fused with a phenyl group.

Three Dimensional Structure of Galactosyltransferases and Ligand Binding Domains of Same

The present invention provides a galactosyltransferase secondary, tertiary and/or quanternary structure. The invention also provides a homology model that represents the secondary, tertiary, and/or quanternary structure of a galactosyltransferase. A model may, for example, be a structural model (or representation thereof), or a computer model. The model itself may be in two or three dimensions. It is possible for a computer model to be in three dimensions despite the constraints imposed by a conventional computer screen, if it is possible to scroll along at least a pair of axes, causing "rotation" of the image.

In accordance with an aspect of the invention a method is provided for designing a homology model of a ligand binding domain of a galactosytransferase wherein the homology model may be displayed as a three-dimensional image, the method comprising:

(i) providing an amino acid sequence and structural coordinates of a ligand binding domain structure of a glycosyltransferase, preferably SpsA glycosytransferase;

(ii) modifying said structure to take into account differences between the amino acid configuration of the ligand binding domains of the galactosyltransferase on the one hand and the SpsA glycosyltransferase on the other hand to generate a homology model, and

(iii) if required refining the homology model.

The method may further comprise comparing the homology model with the structures of other, similar, proteins.

A model or structure of a preferred galactosyltransferase of the invention has the atomic structural coordinates as shown in Table 4 or Table 8. Computer representations of the structure i.e. models are illustrated in the Figures.

The structural coordinates in a structure or model of the invention may comprise the amino acid residues of a galactosyltransferase ligand binding domain, or a portion or homolog thereof useful in the modeling and design of test compounds capable of binding to the galactosyltransferase. Therefore, the invention also relates to a secondary and three dimensional structure or model of a ligand binding domain of a galactosyltransferase. Ligand binding domains include the ligand binding domains for a disphosphate group of a sugar nucleotide donor, a nucleotide of a sugar nucleotide donor, a nitrogeneous heterocyclic base (preferably a pyrimidine base, more preferably uracil) of a sugar nucleotide donor, and/or a sugar (e.g. galactose) of a sugar nucleotide donor. The structure of a ligand binding domain may be defined by selected atomic interactions or contacts in the domain, preferably two or more of the atomic interactions or contacts as defined in Table 1.

It is understood that a structure or model of the invention includes a structure where at least one amino acid residue is replaced with a different amino acid residue or by adding or deleting amino acid residues, and having substantially the same three dimensional structure as the galactosyltransferase as described in Table 4 and the Figures, or the ligand binding domains as described in Table 1 (and further defined by the structural coordinates of the ATOMS in Table 4 or Table 8), i.e. having a set of atomic structural coordinates that have a root mean square deviation of less than or equal to about 2Å, preferably less than 0.5Å, most preferably less than 0.3Å, when superimposed with the atomic structure coordinates of the galactosyltransferase as described in Table 4 or Table 8, or the binding domains as described in Table 1 (and further defined by the structural coordinates of the ATOMS in Table 4) when at least 50% to 100% of the atoms of the sugar nucleotide donor binding domain or binding domains of components of the donor as the case may be, are included in the superimposition.

The invention also features a secondary and three dimensional structure or model of a galactosyltransferase in association with one or more molecules (e.g. substrates such as UDP-Gal, uridine-ribose, monophophate-Mn^{2+}, or diphosphate-Mn^{2+}). The association may be covalent or non-covalent. The molecule may be any organic molecule, and it may modulate the function of a galactosyltransferase by for example inhibiting or enhancing its function, or it may be an acceptor or donor for the galactosyltransferase. It is preferred that the geometry of the compound and the interactions formed between the compound and the galacytosyltransferase provide high affinity binding between the two molecules.

The structure and model of the galactosyltransferase decribed herein has allowed the identification and characterization of the binding domain of UDP and UDP-Gal. The UDP-Gal binding domain has been subdivided into three sub-sites (the uracil-binding domain, the ribose-binding domain, the diphosphate-Mn^{2+} binding domain, and the Gal binding domain) and characterized.

Therefore, in an embodiment of the invention, a secondary and three dimensional structure or model of a ligand binding domain of a galactosyltransferase that binds a diphosphate of a sugar nucleotide donor is provided comprising at least two of atomic interactions 9, 10, and 11 of Table 1, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the diphosphate, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the galactosyltransferase (i.e. enzyme atomic contact). In a preferred embodiment, the ligand binding domain comprises atomic interactions 9 and 10, 10 and 11, 9 and 11, or 9, 10, and 11 of Table 1. Preferably, the binding domain is defined by the atoms of the enzyme atomic interactions having the structural coordinates for the atoms listed in Table 4 or Table 8. Therefore, in an embodiment of the invention the binding domain is defined by the structural coordinates referred to as ATOM 1690, and ATOM 1718 of Table 8most preferably ATOM 1690 to ATOM 1718 inclusive of Table 8. The binding domain of a galactosyltransferase for a diphosphate of a sugar nucleotide donor is also characterized by a DVD motif (Asp-225, Val-226, and Asp-227).

In another embodiment of the invention, a secondary or three dimensional structure or model of a ligand binding domain of a galactosyltransferase that binds a heterocyclic amine base of a sugar nucleotide donor is provided comprising at least two, preferably three, of atomic interactions 1, 2, 3, and 4 of Table 1, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the heterocyclic amine base, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the galactosyltransferase (i.e. enzyme atomic contact). In a preferred embodiment, the ligand binding domain comprises atomic interactions 1 and 2; 1 and 3; 1 and 4; 2 and 3; 2 and 4; 3 and 4; or 1, 2, and 3; 2, 3, and 4; 1, 3,

and 4; 1, 2, and 4; or 1, 2, 3 and 4 of Table 1. Preferably, the binding domain is defined by the atoms of the enzyme atomic interactions having the structural coordinates for the atoms listed in Table 4 or Table 8. Therefore, in an embodiment of the invention the binding domain is defined by the structural coordinates referred to as ATOM 720, ATOM 1360, ATOM 1490, ATOM 154 to ATOM 155 in Table 8. The ligand binding domain of a galactosyltransferase for a heterocyclic amine base of a sugar nucleotide donor is also characterized by two helices and two β sheets in anti-parallel fashion. A ligand binding domain for uracil can also be characterized by the following three hydrogen bonds: (1) the amide hydrogen of uracil in position 3 and OD1 of Asp-168, (2) the carbonyl oxygen of uracil in position 4 and the side chain of Lys-204, and (3) the carbonyl oxygen of uracil in position 2 and the amide hydrogen of the His-213 side chain.

In another embodiment of the invention, a secondary and three dimensional structure or model of a ligand binding domain of a galactosyltransferase that binds the sugar of the nucleotide (e.g. ribose) of a sugar nucleotide donor is provided comprising at least two, preferably three, of atomic interactions 5, 6, 7, and 8 of Table 1, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the sugar, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the galactosyltransferase (i.e. enzyme atomic contact). In a preferred embodiment, the binding domain comprises atomic interactions 5 and 6; 5 and 7; 5 and 8; 6 and 7; 6 and 8; 7 and 8; 5, 6, and 7; 5, 6, and 8; 6, 7, and 8; 5, 7, and 8; and 5, 6, 7,and 8 of Table 1. Preferably, the ligand binding domain is defined by the atoms of the enzyme atomic interactions having the structural coordinates for the atoms listed in Table 4 or Table 8. Therefore, in an embodiment of the invention the binding domain is defined by the structural coordinates referred to as ATOM 1690, ATOM 97 to ATOM 115, ATOM 1436 to ATOM 1454 of Table 8.

Atomic interactions 1 through 11 in Table 1 are preferably each characterized by the types of binding and/or the distances between atomic contacts indicated in Table 1.

In another embodiment of the invention, a secondary or three dimensional structure of a ligand binding domain of a galactosyltransferase that binds a nucleotide (preferably UDP) of a sugar nucleotide donor is provided comprising at least two or more of atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, or 11 of Table 1, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the nucleotide, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the galactosyltransferase (i.e. enzyme atomic contact). In a preferred embodiment, the binding domain comprises atomic interactions 2, 3, 5, 6, , 9, 10, and 11; 4, 7, 8, 9, 10, and 11; 1, 2, 3, 5, 6, 9, 10, 11, or 1 to 11 inclusive of Table 1. Preferably, the ligand binding domain is defined by the atoms of the enzyme atomic interactions having the structural coordinates for the atoms listed in Table 4 or Table 8. Therefore, in an embodiment of the invention the ligand binding domain is defined by the structural coordinates referred to as ATOM 720, ATOM 1360, ATOM 1490, ATOM 154, ATOM 155, ATOM 1690, ATOM 97 to ATOM 115, ATOM 1436 to ATOM 1454, and ATOM 1718, of Table 8. The binding domain of a galactosyltransferase for a nucleotide of a sugar nucleotide donor is also characterized by a 100 amino acid nucleotide recognition domain.

A UDP binding domain of a galactosyltransferase is also characterized by an open α,β-sandwich made up of three helices packed against four β-sheets. The following amino acid residues have also been identified to be part of the UDP binding domain: Phe-134, Typ-139, Ile-140, Val-136, Arg-194, Arg-202, Lys-209, Asp-173, His-218, Thr-137, Asp-225, Val-226, and Asp-227.

In yet another embodiment of the invention, a secondary and three dimensional structure or model of a ligand binding domain of a galactosyltransferase that binds a sugar nucleotide donor (preferably UDP-Gal) is provided comprising at least three of the atomic interactions of Table 1, each atomic interaction defined therein by an atomic contact (more preferably, a specific atom where indicated) on the sugar nucleotide donor, and an atomic contact (more preferably, a specific amino acid residue where indicated) on the galactosyltransferase (i.e. enzyme atomic contact). In a preferred embodiment, the binding domain comprises atomic interactions 1 to 11 inclusive of Table 1. Preferably, the ligand binding domain is defined by the atoms of the enzyme atomic interactions having the structural coordinates for the atoms listed in Table 4 or Table 8. Therefore, in an embodiment of the invention the ligand binding domain is defined by the structural coordinates referred to as ATOM 720, ATOM 1360, ATOM 1490, ATOM 154, ATOM 155, ATOM 1690, ATOM 97 to ATOM 115, ATOM 1436 to ATOM 1454, and ATOM 1718 of Table 4.

Identification of Homologues

The knowledge of the structures and models of the invention enables one skilled in the art to identify homologues of galactosyltransferases. This is achieved by searches of three-dimensional databases. Since structural folds are conserved to a greater extent than sequence, one may identify homologues with very little sequence identity or similarity. Programs that provide this type of database searching are known in the art and include Dal and the Fold recognition server located at UCLA (8). The structural coordinates of a protein structure are submitted and the program performs a multiple structural alignment with proteins in the protein data bank. Homologues identified in accordance with the present invention may be used in the methods of the invention described herein.

Computer Format of Structures/Models

Information derivable from the structures of the present invention (for example the structural coordinates) or a model of the present invention may be provided in a computer-readable format.

Therefore, the invention provides a computer readable medium or a machine readable storage medium which comprises the models of the invention or structural coordinates of a galactosyltransferase including all or any parts of the galactosyltransfersae (e.g ligand-binding domain), ligands including portions thereof, or substrates including portions thereof. Such storage medium or storage medium encoded with these data are capable of displaying on a computer screen or similar viewing device, a three-dimensional graphical representation of a molecule or molecular complex which comprises the enzyme or ligand binding domains or similarly shaped homologous enzymes or ligand binding domains. Thus, the invention also provides computerized representations of a model or structure of the invention, including any electronic, magnetic, or electromagnetic storage forms of the data needed to define the structures such that the data will be computer readable for purposes of display and/or manipulation.

In an aspect the invention provides a computer for producing a model or three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a galactosyltransferase or ligand binding domain thereof defined by structural coordinates of galactosyltransferase amino acids or a ligand binding domain thereof, or comprises structural coordinates of atoms of a ligand or substrate, or a three-dimensional representation of a homologue of said molecule or molecular complex, wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates of a galactosyltransferase

amino acids according to Table 4 or Table 8 or a ligand binding domain thereof, or a ligand according to Table 5, 6, or 7;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

A homologue may comprise a galactosyltransferase or ligand binding domain thereof, or ligand or substrate that has a root mean square deviation from the backbone atoms of not more than 1.5 angstroms.

The invention also provides a computer for determining at least a portion of the structural coordinates corresponding to an X-ray diffraction pattern of a molecule or molecular complex wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates according to Table 4, 5, 6, 7, or 8;

(b) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises an X-ray diffraction pattern of said molecule or molecular complex;

(c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);

(d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structural coordinates; and

(e) a display coupled to said central-processing unit for displaying said structural coordinates of said molecule or molecular complex.

The invention also contemplates a computer programmed with a homology model of a ligand binding domain according to the invention; a machine-readable data-storage medium on which has been stored in machine-readable form a homology model of a ligand binding domain of a galactosyltransferase; and the use of a homology model as input to a computer programmed for drug design and/or database searching and/or molecular graphic imaging in order to identify new ligands for galactosyltransferases.

Structural Determinations

The present invention also provides a method for determining the secondary and/or tertiary structures of a polypeptide by using a model according to the invention. The polypeptide may be any polypeptide for which the secondary and or tertiary structure is uncharacterised or incompletely characterised. In a preferred embodiment the polypeptide shares (or is predicted to share) some structural or functional homology to a galactosyltransferase, preferably a β1,3 galactosyltranferase. For example, the polypeptide may show a degree of structural homology over some or all parts of the primary amino acid sequence. For example the polypeptide may have one or more domains which show homology with a galactosyltransferase domain (Kapitonov and Yu (1999) Glycobiology 9(10): 961-978).

The polypeptide may be a galactosyltransferase with a different specificity for a ligand or substrate. The polypeptide may be a galactosyltransferase which requires a different metal cofactor. Alternatively (or in addition) the polypeptide may be a galactosyltransferase from a different species.

The polypeptide may be a mutant of the wild-type galactosyltransferase. A mutant may arise naturally, or may be made artificially (for example using molecular biology techniques). The mutant may also not be "made" at all in the conventional sense, but merely tested theoretically using the model of the present invention. A mutant may or may not be functional.

Thus, using a model of the present invention, the effect of a particular mutation on the overall two and/or three dimensional structure of a galactosyltransferase and/or the interaction between the enzyme and a ligand or substrate can be investigated. Alternatively, the polypeptide may perform an analogous function or be suspected to show a similar catalytic mechanism to the galactosyltransferase enzyme. For example the polypeptide may transfer a sugar residue from a sugar nucleotide donor.

The polypeptide may also be the same as the polypeptide described herein, but in association with a different ligand (for example, modulator or inhibitor) or cofactor. In this way it is possible to investigate the effect of altering a ligand or compound with which the polypeptide is associated on the structure of a ligand binding domain.

Secondary or tertiary structure may be determined by applying the structural coordinates of the model of the present invention to other data such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Homology modeling, molecular replacement, and nuclear magnetic resonance methods using these other data sets are described below.

Homology modeling (also known as comparative modeling or knowledge-based modeling) methods develop a three dimensional model from a polypeptide sequence based on the structures of known proteins (e.g. native or mutated galactosyltransferases). In the present invention the method utilizes a computer representation of the structure of a galactosyltransferase, or a binding domain or complex of same as described herein, a computer representation of the amino acid sequence of a polypeptide with an unknown structure (additional native or mutated galactosyltransferases), and standard computer representations of the structures of amino acids. The method in particular comprises the steps of; (a) identifying structurally conserved and variable regions in the known structure; (b) aligning the amino acid sequences of the known structure and unknown structure (c) generating coordinates of main chain atoms and side chain atoms in structurally conserved and variable regions of the unknown structure based on the coordinates of the known structure thereby obtaining a homology model; and (d) refining the homology model to obtain a three dimensional structure for the unknown structure. This method is well known to those skilled in the art (Greer, 1985, Science 228, 1055; Bundell et al 1988, Eur. J. Biochem. 172, 513; Knighton et al., 1992, Science 258:130-135, http://biochem.vt.edu/courses/modeling/ homology.htn). Computer programs that can be used in homology modeling are Quanta and the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc, or MODELLER (Rockefeller University, www.iucr.ac.uk/sinris-top/logical/prg-modeller.html).

In step (a) of the homology modeling method, a known galactosyltransferase structure is examined to identify the structurally conserved regions (SCRs) from which an average structure, or framework, can be constructed for these regions of the protein. Variable regions (VRs), in which known structures may differ in conformation, also must be identified. SCRs generally correspond to the elements of secondary structure, such as

alpha-helices and beta-sheets, and to ligand- and substrate-binding sites (e.g. acceptor and donor binding sites). The VRs usually lie on the surface of the proteins and form the loops where the main chain turns.

Many methods are available for sequence alignment of known structures and unknown structures. Sequence alignments generally are based on the dynamic programming algorithm of Needleman and Wunsch [J. Mol. Biol. 48: 442-453, 1970]. Current methods include FASTA, Smith-Waterman, and BLASTP, with the BLASTP method differing from the other two in not allowing gaps. Scoring of alignments typically involves construction of a 20x20 matrix in which identical amino acids and those of similar character (i.e., conservative substitutions) may be scored higher than those of different character. Substitution schemes which may be used to score alignments include the scoring matrices PAM (Dayhoff et al., Meth. Enzymol. 91: 524-545, 1983), and BLOSUM (Henikoff and Henikoff, Proc. Nat. Acad. Sci. USA 89: 10915-10919, 1992), and the matrices based on alignments derived from three-dimensional structures including that of Johnson and Overington (JO matrices) (J. Mol. Biol. 233: 716-738, 1993).

Alignment based solely on sequence may be used, though other structural features also may be taken into account. In Quanta, multiple sequence alignment algorithms are available that may be used when aligning a sequence of the unknown with the known structures. Four scoring systems (i.e. sequence homology, secondary structure homology, residue accessibility homology, CA-CA distance homology) are available, each of which may be evaluated during an alignment so that relative statistical weights may be assigned.

When generating coordinates for the unknown structure, main chain atoms and side chain atoms, both in SCRs and VRs need to be modeled. A variety of approaches may be used to assign coordinates to the unknown. In particular, the coordinates of the main chain atoms of SCRs will be transferred to the unknown structure. VRs correspond most often to the loops on the surface of the polypeptide and if a loop in the known structure is a good model for the unknown, then the main chain coordinates of the known structure may be copied. Side chain coordinates of SCRs and VRs are copied if the residue type in the unknown is identical to or very similar to that in the known structure. For other side chain coordinates, a side chain rotamer library may be used to define the side chain coordinates. When a good model for a loop cannot be found fragment databases may be searched for loops in other proteins that may provide a suitable model for the unknown. If desired, the loop may then be subjected to conformational searching to identify low energy conformers if desired.

Once a homology model has been generated it is analyzed to determine its correctness. A computer program available to assist in this analysis is the Protein Health module in Quanta which provides a variety of tests. Other programs that provide structure analysis along with output include PROCHECK and 3D-Profiler [Luthy R. et al, Nature 356: 83-85, 1992; and Bowie, J.U. et al, Science 253: 164-170, 1991]. Once any irregularities have been resolved, the entire structure may be further refined. Refinement may consist of energy minimization with restraints, especially for the SCRs. Restraints may be gradually removed for subsequent minimizations. Molecular dynamics may also be applied in conjunction with energy minimization.

The structural coordinates of a galactosyltransferase structure may be applied to nuclear magnetic resonance (NMR) data to determine the three dimensional structures of polypeptides in solution (e.g. additional native or mutated galactosyltransferases). (See for example, Wuthrich, 1986, John Wiley and Sons, New York: 176-199; Pflugrath et al., 1986, J. Molecular Biology 189: 383-386; Kline et al., 1986 J. Molecular Biology 189:377-382). While the secondary structure of a polypeptide may often be determined by NMR data, the spatial connections between individual pieces of secondary structure are not as readily determined. The structural coordinates of a polypeptide can guide the NMR spectroscopist to an understanding of the spatical interactions between secondary

structural elements in a polypeptide of related structure. Information on spatial interactions between secondary structural elements can greatly simplify Nuclear Overhauser Effect (NOE) data from two-dimensional NMR experiments. In addition, applying the structural coordinates after the determination of secondary structure by NMR techniques simplifies the assignment of NOE's relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure.

In an embodiment, the invention relates to a method of determining three dimensional structures of polypeptides with unknown structures, preferably a native or mutated galactosyltransferases, by applying the structural coordinates of a galactosyltransferase structure, or ligand binding domain or complex thereof described herein to nuclear magnetic resonance (NMR) data of the unknown structure. This method comprises the steps of: (a) determining the secondary structure of an unknown structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The term " through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence. The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

Screening Method

The present invention provides a method of screening for a ligand that associates with a ligand binding domain and/or modulates the function of a galactosyltranssferase, by using a structure or a model according to the present invention. The method may involve investigating whether a test compound is capable of associating with or binding a ligand binding domain.

In accordance with an aspect of the present invention, a method is provided for screening for a ligand capable of associating with or binding to a ligand binding domain, wherein said method comprises the use of a structure or model according to the invention.

In another aspect, the invention relates to a method of screening for a ligand capable of associating with or binding to a ligand binding domain, wherein the ligand binding domain is defined by the amino acid residue structural coordinates given herein, the method comprising contacting the ligand binding domain with a test compound and determining if said test compound binds to said ligand binding domain.

In one embodiment, the present invention provides a method of screening for a test compound capable of interacting with a key amino acid residue of a ligand binding domain of a galactosyltransferase.

Another aspect of the invention provides a process comprising the steps of:

(a) performing the method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to a ligand binding domain; and

(c) preparing a quantity of said one or more ligands.

A further aspect of the invention provides a process comprising the steps of:

(a) performing the method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to a ligand binding domain; and

(c) preparing a pharmaceutical composition comprising said one or more ligands.

Once a test compound capable of interacting with a key amino acid residue in a galactosyltransferase ligand binding domain has been identified, further steps may be carried out either to select and/or to modify compounds and/or to modify existing compounds, to modulate the interaction with the key amino acid residues in the galactosyltransferase ligand binding domain.

Yet another aspect of the invention provides a process comprising the steps of:

(a) performing the method of screening for a ligand as described above;

(b) identifying one or more ligands capable of binding to a ligand binding domain;

(c) modifying said one or more ligands capable of binding to a ligand binding domain;

(d) performing said method of screening for a ligand as described above;

(e) optionally preparing a pharmaceutical composition comprising said one or more ligands.

As used herein, the term "test compound" means any compound which is potentially capable of associating with a ligand binding domain. If, after testing, it is determined that the test compound does associate with or bind to the ligand binding domain, it is known as a "ligand".

A "test compound" includes, but is not limited to, a compound which may be obtainable from or produced by any suitable source, whether natural or not. The test compound may be designed or obtained from a library of compounds which may comprise peptides, as well as other compounds, such as small organic molecules and particularly new lead compounds. By way of example, the test compound may be a natural substance, a biological macromolecule, or an extract made from biological materials such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic test compound, a semi-synthetic test compound, a carbohydrate, a monosaccharide, an oligosaccharide or polysaccharide, a glycolipid, a glycopeptide, a saponin, a heterocyclic compound, a structural or functional mimetic, a peptide, a peptidomimetic, a derivatised test compound, a peptide cleaved from a whole protein, or a peptide synthesised synthetically (such as, by way of example, either using a peptide synthesizer or by recombinant techniques or combinations thereof), a recombinant test compound, a natural or a non-natural test compound, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof.

The test compound may be screened as part of a library or a data base of molecules. Data bases which may be used include ACD (Molecular Designs Limited), NCI (National Cancer Institute), CCDC (Cambridge Crystallographic Data Center), CAST (Chemical Abstract Service), Derwent (Derwent Information Limited), Maybridge (Maybridge Chemical Company Ltd), Aldrich (Aldrich Chemical Company), DOCK (University of California in San Francisco), and the Directory of Natural Products (Chapman & Hall). Computer programs such as CONCORD (Tripos Associates) or DB-Converter (Molecular Simulations Limited) can be used to convert a data set represented in two dimensions to one represented in three dimensions.

Test compounds may be tested for their capacity to fit spatially into a galactosyltransferase ligand binding domain. As used herein, the term "fits spatially" means that the three-dimensional structure of the test compound is accommodated geometrically in a galactosyltransferase ligand binding domain. The test compound can then be considered to be a ligand.

A favourable geometric fit occurs when the surface area of the test compound is in close proximity with the surface area of the cavity or pocket without forming unfavorable interactions or associations. A favourable complementary interaction occurs where the test compound interacts by hydrophobic, aromatic, ionic, dipolar, or hydrogen donating and accepting forces. Unfavourable interactions or associations may be steric hindrance between atoms in the test compound and atoms in the binding site.

In an embodiment of the invention, a method is provided for identifying potential modulators of galactosyltransferase function. The method utilizes the structural coordinates or model of a galactosyltransferase three dimensional structure, or binding domain thereof. The method comprises the steps of (a) docking a computer

representation of a test compound from a computer data base with a computer model of a ligand binding domain of a galactosyltransferase; (b) determining a conformation of a complex between the test compound and binding domain with a favourable geometric fit or favorable complementary interactions; and (c) identifying test compounds that best fit the galactosyltransferase binding domain as potential modulators of galactosyltransferase function. The initial galactosyltransferase structure may or may not have substrates bound to it. A favourable complementary interaction occurs where a compound in a compound-galactosyltransferase complex interacts by hydrophobic, ionic, or hydrogen donating and accepting forces, with the active-site or ligand binding domain of a galactosyltransferase without forming unfavorable interactions.

If a model of the present invention is a computer model, the test compounds may be positioned in a ligand binding domain through computational docking. If, on the other hand, the model of the present invention is a structural model, the test compounds may be positioned in the ligand binding domain by, for example, manual docking.

As used herein the term "docking" refers to a process of placing a compound in close proximity with a galactosyltransferase ligand binding domain, or a process of finding low energy conformations of a test compound/ galactosyltransferase complex.

A screening method of the present invention may comprise the following steps:

(i) generating a computer model of a galactosyltransferase or a ligand binding domain thereof according to the first aspect of the invention;

(ii) docking a computer representation of a test compound with the computer model;

(iii) analysing the fit of the compound in the galactosyltransferase or ligand binding domain thereof.

In an aspect of the invention a method is provided comprising the following steps:

(a) docking a computer representation of a structure of a test compound into a computer representation of a ligand binding domain of a galactosyltransferase defined in accordance with the invention using a computer program, or by interactively moving the representation of the test compound into the representation of the binding domain;

(b) characterizing the geometry and the complementary interactions formed between the atoms of the ligand binding domain and the test compound; optionally

(c) searching libraries for molecular fragments which can fit into the empty space between the compound and ligand binding domain and can be linked to the compound; and

(d) linking the fragments found in (c) to the compound and evaluating the new modified compound.

In an embodiment of the invention a method is provided which comprises the following steps:

(a) docking a computer representation of a test compound from a computer data base with a computer representation of a selected site (e.g. an inhibitor binding domain) on a galactosyltransferase structure or model defined in accordance with the invention to obtain a complex;

(b) determining a conformation of the complex with a favourable geometric fit and favourable complementary interactions; and

(c) identifying test compounds that best fit the selected site as potential modulators of the galactosyltransferase.

A method of the invention may be applied to a plurality of test compounds, to identify those that best fit the selected site.

The model used in the screening method may comprise a galactosyltransferase or ligand binding domain thereof either alone or in association with one or more ligands and/or cofactors. For example, the model may comprise the ligand-binding domain in association with a ligand, substrate, or analogue thereof.

If the model comprises an unassociated ligand binding domain, then the selected site under investigation may be the ligand binding domain itself. The test compound may, for example, mimic a known substrate for the enzyme in order to interact with the ligand binding domain. The selected site may alternatively be another site on the enzyme.

If the model comprises an associated ligand binding domain, for example a ligand binding domain in association with a ligand or substrate molecule or analogue thereof, the selected site may be the ligand binding domain or a site made up of the ligand binding domain and the complexed ligand, or a site on the ligand itself. The test compound may be investigated for its capacity to modulate the interaction with the associated molecule.

A test compound (or plurality of test compounds) may be selected on the basis of its similarity to a known ligand for the galactosyltransferase. For example, the screening method may comprise the following steps:

(i) generating a computer model of a galactosyltransferase ligand binding domain in complex with a ligand;

(ii) searching for a test compound with a similar three dimensional structure and/or similar chemical groups; and

(iii) evaluating the fit of the test compound in the ligand binding domain.

Searching may be carried out using a database of computer representations of potential compounds, using methods known in the art.

The present invention also provides a method for designing ligands for a galactosyltransferase. It is well known in the art to use a screening method as described above to identify a test compound with promising fit, but then to use this test compound as a starting point to design a ligand with improved fit to the model. A known modulator can also be modified to enhance its fit with a model of the invention. Such techniques are known as "structure–based ligand design" (See Kuntz et al., 1994, Acc. Chem. Res. 27:117; Guida, 1994, Current Opinion in Struc. Biol. 4: 777; and Colman, 1994, Current Opinion in Struc. Biol. 4: 868, for reviews of structure-based drug design and identification;and Kuntz et al 1982, J. Mol. Biol. 162:269; Kuntz et al., 1994, Acc. Chem. Res. 27: 117; Meng et al., 1992, J. Compt. Chem. 13: 505; Bohm, 1994, J. Comp. Aided Molec. Design 8: 623 for methods of structure-based modulator design).

Examples of computer programs that may be used for structure-based ligand design are CAVEAT (Bartlett et al., 1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M. Ley, S.V.; Campbell, N.M. eds; Royal Society of Chemistry: Cambridge, pp 182-196); FLOG (Miller et al., 1994, J. Comp. Aided Molec. Design 8:153); PRO Modulator (Clark et al., 1995 J. Comp. Aided Molec. Design 9:13); MCSS (Miranker and Karplus, 1991, Proteins: Structure, Function, and Genetics 8:195); and, GRID (Goodford, 1985, J. Med. Chem. 28:849).

The method may comprise the following steps:

(i) docking a model of a test compound with a model of a selected ligand binding domain;

(ii) identifying one or more groups on the test compound which may be modified to improve their fit in the selected ligand binding domain;

(iii) replacing one or more identified groups to produce a modified test compound model; and

(iv) docking the modified test compound model with the model of the selected ligand binding domain.

Evaluation of fit may comprise the following steps:

(a) mapping chemical features of a test compound such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites; and

(b) adding geometric constraints to selected mapped features.

The fit of the modified test compound may then be evaluated using the same criteria.

The chemical modification of a group may either enhance or reduce hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between the test compound and the key amino acid residue(s) of the selected site. Preferably the group modifications involve the addition, removal, or replacement of substituents onto the test compound such that the substituents are positioned to collide or to bind preferentially with one or more amino acid residues that correspond to the key amino acid residues of the selected site.

Identified groups in a test compound may be substituted with, for example, alkyl, alkoxy, hydroxyl, aryl, cycloalkyl, alkenyl, alkynyl, thiol, thioalkyl, thioaryl, amino, or halo groups. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided.

If a modified test compound model has an improved fit, then it may bind to the selected site and be considered to be a "ligand". Rational modification of groups may be made with the aid of libraries of molecular fragments which may be screened for their capacity to fit into the available space and to interact with the appropriate atoms. Databases of computer representations of libraries of chemical groups are available commercially, for this purpose.

A test compound may also be modified "*in situ*" (i.e. once docked into the potential binding domain), enabling immediate evaluation of the effect of replacing selected groups. The computer representation of the test compound may be modified by deleting a chemical group or groups, replacing chemical groups, or by adding a chemical group or groups. After each modification to a compound, the atoms of the modified compound and potential binding site can be shifted in conformation and the distance between the modulator and the active site atoms may be scored on the basis of geometric fit and favourable complementary interactions between the molecules. This technique is described in detail in Molecular Simulations User Manual, 1995 in LUDI.

Examples of ligand building and/or searching computer programs include programs in the Molecular Simulations Package (Catalyst), ISIS/HOST, ISIS/BASE, and ISIS/DRAW (Molecular Designs Limited), and UNITY (Tripos Associates).

The "starting point" for rational ligand design may be a known ligand for the enzyme. For example, in order to identify potential modulators of a galactosyltransferase, a logical approach would be to start with a known ligand (for example a substrate molecule or inhibitor) to produce a molecule which mimics the binding of the ligand. Such a molecule may, for example, act as a competitive inhibitor for the true ligand, or may bind so strongly that the interaction (and inhibition) is effectively irreversible. Such a method may comprise the following steps:

(i) generating a computer model of a galactosyltransferase ligand binding domain in complex with a ligand;

(ii) replacing one or more groups on the ligand computer model to produce a modified ligand; and

(iii) evaluating the fit of the modified ligand in the ligand binding domain.

The replacement groups could be selected and replaced using a compound construction program which replaces computer representations of chemical groups with groups from a computer database, where the representations of the compounds are defined by structural coordinates.

In an embodiment, a screening method is provided for identifying a ligand of a galactosyltransferase comprising the step of using the structural coordinates or model of a substrate molecule or component thereof, defined in relation to its spatial association with a galactosyltransferase structure or a ligand binding domain, to generate a compound that is capable of associating with the galactosyltransferase or ligand binding domain.

The invention contemplates a method for the design of modulators for galactosyltransferases based on the three dimensional structure or model of a sugar nucleotide donor (or parts thereof) defined in relation to the three dimensional structure of a ligand binding domain.

In accordance with particular aspects of the invention, a method is provided for designing potential inhibitors of a galactosyltransferase comprising the step of using the structural coordinates of uracil, uridine, or UDP of Table 5, 6, or 7 to generate a compound for associating with the active site of a ligand binding domain of a galactosyltransferase. The following steps are employed in a particular method of the invention: (a) generating a computer representation of uracil, uridine, or UDP defined by structural coordinates of Table 5, 6 or 7; (b) searching for molecules in a data base that are similar to the defined uracil, uridine, or UDP using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

In another embodiment of the invention, a method is provided for designing potential inhibitors of a glycosyltransferase comprising the step of using the structural coordinates of UDP-Gal of Table 6, to generate a compound for associating with the active site of a galactosyltransferase. The following steps are employed in a particular method of the invention: (a) generating a computer representation of UDP-Gal defined by the structural coordinates of Table 6; (b) searching for molecules in a data base that are similar to the defined UDP-Gal using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

The screening methods of the present invention may be used to identify compounds or entities that associate with a molecule that associates with a galactosyltransferase enzyme (for example, a substrate molecule).

Compounds and entities (e.g. ligands) of a galactosyltransferase identified using the above-described methods may be prepared using methods described in standard reference sources utilized by those skilled in the art. For example, organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill. (See detailed discussion herein.)

Test compounds and ligands which are identified using a model of the present invention can be screened in assays such as those well known in the art. Screening can be, for example, *in vitro*, in cell culture, and/or *in vivo*. Biological screening assays preferably centre on activity-based response models, binding assays (which measure how well a compound binds), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity-high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity. The biological assay,

may also be an assay for the ligand binding activity of a compound that selectively binds to the ligand binding domain compared to other enzymes.

Ligands/Modulators

The present invention provides a ligand or compound or entity identified by a screening method of the present invention. A ligand or compound may have been designed rationally by using a model according to the present invention. A ligand or compound identified using the screening methods of the invention specifically associate with a target compound. In the present invention the target compound may be a galactosyltransferase or a molecule that is capable of associating with a galactosyltransferase (for example a substrate molecule). In a preferred embodiment the ligand is capable of binding to the ligand binding domain of a galactosyltransferase.

A ligand or compound identified using a screening method of the invention may act as a "modulator", i.e. a compound which affects the activity of a galactosyltransferase. A modulator may reduce, enhance or alter the biological function of a galactosyltransferase. For example a modulator may modulate the capacity of the enzyme to transfer a sugar from a nucleotide sugar donor to a specific hydroxyl of various saccharide acceptors that leads to the formation of a new glycosidic linkage. An alteration in biological function may be characterised by a change in specificity. For example, a modulator may cause the enzyme to accept a different substrate molecule, to transfer a different sugar, or to work with a different metal cofactor. In order to exert its function, the modulator commonly binds to the ligand binding domain.

A modulator which is capable of reducing the biological function of the enzyme may also be known as an inhibitor. Preferably an inhibitor reduces or blocks the capacity of the enzyme to form new glycosidic linkages. The inhibitor may mimic the binding of a substrate molecule, for example, it may be a substrate analogue. A substrate analogue may be designed by considering the interactions between the substrate molecule and the enzyme (for example by using information derivable from a model of the invention) and specifically altering one or more groups.

In a highly preferred embodiment, a modulator acts as an inhibitor of a galactosyltransferase and is capable of inhibiting N- or O-glycan biosynthesis.

The present invention also provides a method for modulating the activity of a galactosyltransferase within a cell using a modulator according to the present invention. It would be possible to monitor the expression of N-glycans on the cell surface following such treatment by a number of methods known in the art (for example by detecting expression with an N-and O-glycan specific antibody).

In another preferred embodiment, the modulator modulates the catalytic mechanism of the enzyme.

A modulator may be an agonist, partial agonist, partial inverse agonist or antagonist of a galactosyltransferase or a ligand binding domain.

The term "agonist" includes any ligand, which is capable of binding to a ligand binding domain and which is capable of increasing a proportion of active enzyme, resulting in an increased biological response. The term includes partial agonists and inverse agonists.

The term "partial agonist" includes an agonist that is unable to evoke the maximal response of a biological system, even at a concentration sufficient to saturate a specific ligand binding domain.

The term "partial inverse agonist" includes an inverse agonist that evokes a submaximal response to a biological system, even at a concentration sufficient to saturate a specific ligand binding domain. At high concentrations, it will diminish the actions of a full inverse agonist.

The invention relates to a galactosyltransferase ligand binding domain antagonist, wherein said ligand binding domain is that defined by the amino acid structural coordinates described herein. For example the ligand may antagonise the inhibition of galactosyltransferase by an inhibitor.

The term "antagonist" includes any agent that reduces the action of another agent, such as an agonist. The antagonist may act at the same site as the agonist (competitive antagonism). The antagonistic action may result from a combination of the substance being antagonised (chemical antagonism) or the production of an opposite effect through a different binding site (functional antagonism or physiological antagonism) or as a consequence of competition for the binding site of an intermediate that links the enzyme to the effect observed (indirect antagonism).

The term "competitive antagonism" refers to the competition between an agonist and an antagonist for a ligand binding domain that occurs when the binding of agonist and antagonist becomes mutually exclusive. This may be because the agonist and antagonist compete for the same binding site or combine with adjacent but overlapping sites. A third possibility is that different sites are involved but that they influence the same macromolecules in such a way that agonist and antagonist molecules cannot be bound at the same time. If the agonist and antagonist form only short lived combinations with the binding site so that equilibrium between agonist, antagonist and binding site is reached during the presence of the agonist, the antagonism will be surmountable over a wide range of concentrations. In contrast, some antagonists, when in close enough proximity to their binding site, may form a stable covalent bond with it and the antagonism becomes insurmountable when no spare receptors remain.

As mentioned above, an identified ligand or compound may act as a ligand model (for example, a template) for the development of other compounds. A modulator may be a mimetic of a ligand or ligand binding domain. A mimetic of a ligand may compete with a natural ligand for a galactosyltransferase and antagonize a physiological effect of the enzyme in an animal. A mimetic of a ligand may be an organically synthesized compound. A mimetic of a ligand binding domain, may be either a peptide, polysaccharide, oligosaccharide, or other biopharmaceutical (such as an organically synthesized compound) that specifically binds to a natural substrate molecule for a galactosyltransferase and antagonize a physiological effect of the enzyme in an animal.

Once a ligand has been optimally selected or designed, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to a galactosyltransfease ligand binding domain by the same computer methods described above.

Preferably, positions for substitution are selected based on the predicted binding orientation of a ligand to a galactosyltransferase ligand binding domain.

A technique suitable for preparing a modulator will depend on its chemical nature. For example, organic compounds may be prepared by organic synthetic methods described in references such as March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, New York, McGraw Hill. Peptides can be synthesized by solid phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 43 1 A Peptide Synthesizer (Perkin Elmer) in accordance with the instructions provided by the manufacturer. Once cleaved from the resin, the peptide may be purified by preparative high performance liquid chromatography (e.g., Creighton (1983) Proteins Structures and Molecular Principles, WH

Freeman and Co, New York NY). The composition of the synthetic peptides may be confirmed by amino acid analysis or sequencing (e.g., the Edman degradation procedure; Creighton, *supra*).

If a modulator is a nucleotide, or a polypeptide expressable therefrom, it may be synthesized, in whole or in part, using chemical methods well known in the art (see Caruthers MH *et al* (1980) Nuc Acids Res Symp Ser 215-23, Horn T *et al* (1980) Nuc Acids Res Symp Ser 225-232), or it may be prepared using recombinant techniques well known in the art.

Direct synthesis of a ligand or mimetics thereof can be performed using various solid-phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 43 1 A Peptide Synthesizer (Perkin Elmer) in accordance with the instructions provided by the manufacturer. Additionally, the amino acid sequences obtainable from the ligand, or any part thereof, may be altered during direct synthesis and/or combined using chemical methods with a sequence from other subunits, or any part thereof, to produce a variant ligand.

In an alternative embodiment of the invention, the coding sequence of a ligand or mimetics thereof may be synthesized, in whole or in part, using chemical methods well known in the art (see Caruthers MH *et al* (1980) Nuc Acids Res Symp Ser 215-23, Horn T *et al* (1980) Nuc Acids Res Symp Ser 225-232).

A wide variety of host cells can be employed for expression of the nucleotide sequences encoding a ligand of the present invention. These cells may be both prokaryotic and eukaryotic host cells. Suitable host cells include bacteria such as *E. coli*, yeast, filamentous fungi, insect cells, mammalian cells, typically immortalized, e.g., mouse, CHO, human and monkey cell lines and derivatives thereof. Preferred host cells are able to process the expression products to produce an appropriate mature polypeptide. Processing includes but is not limited to glycosylation, ubiquitination, disulfide bond formation and general post-translational modification.

In an embodiment of the present invention, the ligand may be a derivative of, or a chemically modified ligand. The term "derivative" or "derivatised" as used herein includes the chemical modification of a ligand.

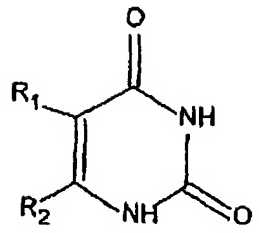
A chemical modification of a ligand and/or a key amino acid residue of a ligand binding domain of the present invention may either enhance or reduce hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between the ligand and the key amino acid residue(s) of a galactosyltransferase ligand binding domain.

Preferably such modifications involve the addition of substituents onto a test compound such that the substituents are positioned to collide or to bind preferentially with one or more amino acid residues that correspond to the key amino acid residues of a galactosyltransferase ligand binding domain. Typical modifications may include, for example, the replacement of a hydrogen by a halo group, an alkyl group, an acyl group or an amino group.

The invention also relates to classes of modulators of galactosyltransferase based on the structure and shape of a substrate, defined in relation to the substrate's molecule's spatial association with a galactosyltransferase structure of the invention or part thereof. Therefore, a modulator may comprise a substrate molecule having the shape or structure, preferably the structural coordinates, of a substrate molecule in an active site binding pocket of a reaction catalyzed by a galactosyltransferase.

Modulators Based on the 3D Structure of a Nucleotide Sugar Donor

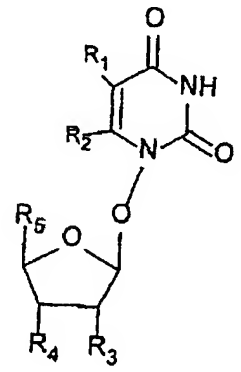
One class of modulators defined by the invention are compounds of the following formula I having the structural coordinates of uracil of Table 5, preferably Run 9, Cluster 1 or ATOM 1 to ATOM 9, inclusive of Table 7:



wherein R_1 and R_2 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, pyrophophate, gallic acid, phosphonates, thioamide, and $-OR_{12}$ where R_{12} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring;

and salts and optically active and racemic forms of a compound of the formula I.

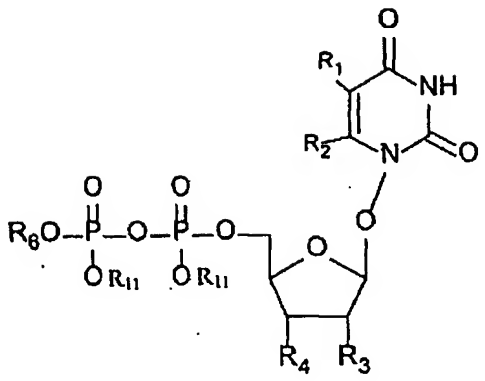
Another class of modulators defined by the invention are compounds of the following formula II having the structural coordinates of uridine of Table 5, preferably Run 9, Cluster 1 or ATOMs 1 to 20 inclusive, of Table 7:



wherein R_1, R_2, R_3, R_4, and R_5 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, pyrophosphate, gallic acid, phosphonates, thioamide, and $-OR_{12}$ where R_{12} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring,

and salts and optically active and racemic forms of a compound of the formula II.

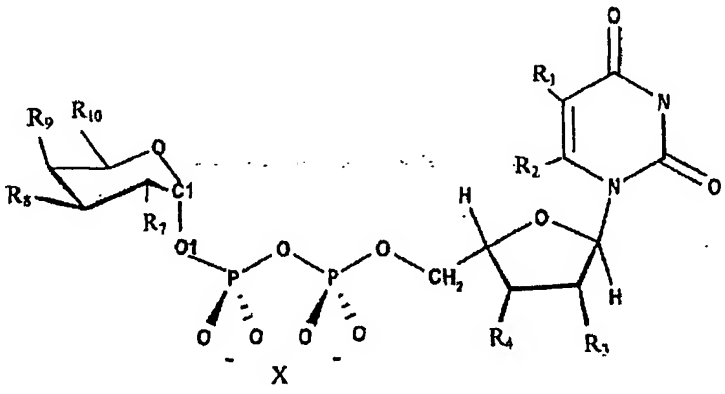
Yet another class of modulators defined by the invention are compounds of the following formula III having the structural coordinates of UDP in Table 5, preferably Run 9, Cluster 1, or ATOMs 1 to 28 inclusive of Table 7:



wherein R_1, R_2, R_3, R_4, R_6, and R_{11} are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, gallic acid, phosphonates, thioamide, and $-OR_{12}$ where R_{12} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring, R_6 may be a monosaccharide or disaccharide, preferably a monosaccharide, including galactose, glucose, and mannose,

and salts and optically active and racemic forms of a compound of the formula III.

Yet another class of modulators defined by the invention are compounds of the following formula IV having the structural coordinates of UDP-Gal in Table 6, preferably Run, Cluster 1:



wherein R_1, R_2, R_3, R_4, R_7, R_8, R_9, and R_{10} are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof (e.g. $-CH_2OH$), amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, gallic acid, phosphonates, thioamide, and $-OR_{12}$ where R_{12} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring, and X is a counter-ion including sodium, lithium, potassium, calcium, magnesium, manganese, cobalt ions and the like, as well as nontoxic ammonium, quaternary ammonium, and amine cations, preferably Mn^{2+},

and salts and optically active and racemic forms of a compound of the formula IV.

One or more of R_1, R_2, R_3, R_4, R_5, R_6, R_7, R_8, R_9, and/or R_{10} alone or together, which contain available functional groups as described herein, may be substituted with for example one or more of the following: alkyl, alkoxy, hydroxyl, aryl, cycloalkyl, alkenyl, alkynyl, thiol, thioalkyl, thioaryl, amino, or halo. The term "one or more" used herein preferably refers to from 1 to 2 substituents.

The present invention contemplates all optical isomers and racemic forms thereof of the compounds of the invention, and the formulas of the compounds shown herein are intended to encompass all possible optical isomers of the compounds so depicted.

The present invention also contemplates salts and esters of the compounds of the invention. In particular, the present invention includes pharmaceutically acceptable salts. By pharmaceutically acceptable salts is meant those salts which are suitable for use in contact with the tissues of humans and lower animals without undue toxicity, irritation, allergic response and the like, and are commensurate with a reasonable benefit/risk ratio. Pharmaceutically acceptable salts are well known in the art and are described for example, in S. M. Berge, et al., J. Pharmaceutical Sciences, 1977, 66:1-19.

Compositions and Methods of Treatment

The ligands and the modulators of the invention (e.g. inhibitors) may be used to modulate the biological activity of a galactosyltransferase in a cell, including modulating a pathway in a cell regulated by the galactosyltransferase or modulating a galactosyltransferase with inappropriate activity in a cellular organism.

The present invention thus provides a method for treating a condition in a subject regulated by a galactosyltransferase or involving inapproproriate galactosyltransferase activity comprising administering to a subject an effective amount of a modulator identified using the methods of the invention. The invention still further relates to a pharmaceutical composition which comprises a three dimensional galactosyltransferase of the invention or a portion thereof (e.g. a ligand binding domain), or a modulator of the invention in an amount effective to regulate one or more of the above-mentioned conditions and a pharmaceutically acceptable carrier, diluent or excipient.

The invention also provides the use of a ligand or modulator according to the invention in the manufacture of a medicament to treat and/or to prevent a disease in a patient.

Inhibitors or antagonists of α1,3-Gal transferase of the present invention may be particularly useful in reducing xenotransplant rejection in an animal patient. Xenograft tissue may be treated with, or derived from an animal that has been treated with an inhibitor to decrease Galα(1,3) Gal epitopes on the xenograft tissue. This treatment will reduce or avoid an immune reaction between circulating antibodies in the transplant recipient reactive with the epitopes. Preferably the xenograft tissue is of pig origin and the xenograft recipient is a human. The xenograft tissue includes any tissue which expresses antigens having Galα(1,3)Gal epitopes. The tissue may be in the form of an organ, for example a kidney, heart, lung, or liver, or it may be in the form of parts of organs, cell clusters, glands and the like (e.g. lenses, pancreatic islet cells, skin, and corneal tissue).

The modulators of the invention may be converted using customary methods into pharmaceutical compositions. The pharmaceutical compositions contain the modulators either alone or together with other active substances. Such pharmaceutical compositions can be for oral, topical, rectal, parenteral, local, inhalant, or intracerebral use. They are therefore in solid or semisolid form, for example pills, tablets, creams, gelatin capsules, capsules, suppositories, soft gelatin capsules, liposomes (see for example, U.S. Patent Serial No. 5,376,452), gels, membranes, and tubelets. For parenteral and intracerebral uses, those forms for intramuscular or subcutaneous administration can be used, or forms for infusion or intravenous or intracerebral injection can be used, and can

therefore be prepared as solutions of the modulators or as powders of the modulators to be mixed with one or more pharmaceutically acceptable excipients or diluents, suitable for the aforesaid uses and with an osmolarity which is compatible with the physiological fluids. For local use, those preparations in the form of creams or ointments for topical use or in the form of sprays should be considered; for inhalant uses, preparations in the form of sprays should be considered.

The pharmaceutical compositions can be prepared by per se known methods for the preparation of pharmaceutically acceptable compositions which can be administered to patients, and such that an effective quantity of the active substance is combined in a mixture with a pharmaceutically acceptable vehicle. Suitable vehicles are described, for example, in Remington's Pharmaceutical Sciences (Remington's Pharmaceutical Sciences, Mack Publishing Company, Easton, Pa., USA 1985). On this basis, the pharmaceutical compositions include, albeit not exclusively, the modulators in association with one or more pharmaceutically acceptable vehicles or diluents, and contained in buffered solutions with a suitable pH and iso-osmotic with the physiological fluids.

The modulators may be indicated as therapeutic agents either alone or in conjunction with other therapeutic agents or other forms of treatment. By way of example, inhibitors may be used in combination with anti-proliferative agents, antimicrobial agents, immunostimulatory agents, or anti-inflammatories. The modulators may be administered concurrently, separately, or sequentially with other therapeutic agents or therapies.

The compositions containing modulators can be administered for prophylactic and/or therapeutic treatments. In therapeutic applications, compositions are administered to a patient already suffering from a condition as described above, in an amount sufficient to cure or at least alleviate the symptoms of the disease and its complications. An amount adequate to accomplish this is defined as a "therapeutically effective dose". Amounts effective for this use will depend on the severity of the disease, the weight and general state of the patient, the nature of the administration route, the nature of the formulation, and the time or interval at which it is administered.

In prophylactic applications, compositions containing modulators are administered to a patient susceptible to or otherwise at risk of a particular condition. Such an amount is defined to be a "prophylactically effective dose". In this use, the precise amounts depend on the patient's state of health and weight, the nature of the administration route, the nature of the formulation, and the time or interval at which it is administered.

The following non-limiting examples illustrate the invention:

Example 1

The modeling of bovine α-1,3-GalT was carried out using homology modeling procedures and α-1,3-GalT-ligand complexes were generated using automated docking procedures. These computational modeling approaches allow fairly reasonable predictions of three-dimensional structures of proteins and their complexes with substrates and ligands thereby offering a rational way of investigating structure-function relationships (12). The amino acid sequence of α-1,3-GalT was obtained from a publicly available sequence data bank (13).

Homology modeling. - The basic steps in the construction of a protein model based on a homologous structure are sequentially in the following order: amino acid sequence alignment, copying aligned coordinates, building loops, and refinement. The sequence alignment and secondary structure predictions were carried out using the Fold recognition server located at UCLA (14). The Molecular Simulations Inc. collection of programs was used for all protein modeling (15-17). The template structure chosen was the three-dimensional crystal structure (9) of SpsA determined at a resolution of 1.5 Å. The initial alignment of α-1,3-GalT and SpsA transferase sequences was obtained using the pair-wise alignment with the HOMOLOGY program (15). Multiple alignment of amino acid sequences was

performed using the Needleman and Wunch method (18). This method is capable to provide an optimum alignment of two sequences that represents the best overall balance between the number of good amino acid matches and the least number of required gaps. When necessary, the initial pair-wise sequence alignments were manually modified to obtain structure-oriented alignments. After creating the alignment, the coordinates of the homologous regions were transferred from the SpsA structure to the bovine α-1,3-GalT using the MODELER program (16). The geometry of the generated model was then locally optimized to remove steric side-chain clashes. The builder module of the InsightII program (17) was used to add hydrogen atoms to the enzyme and assign partial charges.

Docking. - Structures of α-1,3-GalT complexes with UDP, UDP-Gal, and a recently design inhibitor (19) were determined using the AutoDock suite of programs (20), which finds favorable docked configurations for a ligand in a protein-binding site starting from in an arbitrary conformation, orientation and position of a ligand molecule. AutoDock combines conformational search methods such as genetic algorithm and stochastic algorithm with a grid based energy calculation using molecular mechanics type force field, including electrostatic, hydrogen bonding, dispersion/repulsion, and solvation and entropic terms. The overall interaction between the enzyme and ligands were computed using the Amber-like force field as implemented in AutoDock (20). A Mn^{2+} cation position was located, based on the SpsA structure, near the side chain of the Asp227, which belongs to the aspartate-valine-aspartate (DVD) sequence motif. An aspartate-any residue-aspartate (DXD) or the aspartate-any residue-histidine (DXH) motif is common to many glycosyl transferases (21) and is involved in binding metal cations as well as its substrate. Water molecules were not considered in these computations. Positions of all protein atoms were fixed during the docking. The dihedral angles of all ligands were optimized while bond lengths and bond angles were restrained to standard values. Starting structure of UDP was obtained from SpsA-UDP complex and the UDP-Gal was generated using InsightII (17). The conformation of the ribose, galactose and uracil rings were fixed during the docking. In the present work a genetic algorithm was used as the search method. One hundred docking runs were performed for generating complexes of α-1,3-GalT with each of the chosen ligands. For each docking simulation, the population size was set to 50 and 27,000 generations were run. The docked models are clustered using a root mean square tolerance value of 1.5 Å. This approach has been successfully used for a wide variety of structural problems and has been fully described elsewhere (20).

Results and Discussions

Homology model of α-1,3-GalT. - The amino acid sequence alignment of α-1,3-GalT with SpsA and homologous proteins are shown in Figure 1. The highest scoring alignment shows about 40% similarity and 20% identity (45 amino acids are identical). The amino acid residues of SpsA that interact with UDP or located within the UDP binding site are underlined. A clear sequence similarity can be noticed at the active site regions of SpsA and the corresponding aligned residues of α-1,3-GalT. In this figure it can be seen that the residues are well conserved in the region that encompasses the putative UDP binding pocket of SpsA. Table 3 shows the predicted secondary structures for the α-1,3-GalT sequence that was used for generating a homology model of α-1,3-GalT.

The homology model of α-1,3-GalT consists of two compact domains. The predicted N-terminal domain has about 100 residues starting at Gln-125 and ends at Gln-231 and the C-terminus domain has the remaining modeled residues. Figure 2 shows a superposition of the α-1,3-GalT model (blue) and the corresponding SpsA structure (magenta). The amino acid residues of SpsA that interact with the UDP ligand are shown as tubes. The corresponding amino acid residues of α-1,3-GalT are shown as thin tubes. In addition to this overlap at the active site, several exo-

site residues are homologous and placed in similar positions in the three-dimensional space. It can be seen from Figure 2 that the modeled α-1,3-GalT is a compact structure similar to that of SpsA. The overall size of the model of α-1,3-GalT is about 50 Å x 45 Å x 40 Å. The (ϕ,ψ) angles of the constructed model are well within the allowed region of the Ramachandran maps (22). The UDP binding site is identified at the cleft between the strands of conserved residues and an alpha helix within this domain. This site is very deep and is highly electronegative in nature. The active site consists of an open α,β-sandwich made up of three helices packed against four standard β-sheets. The general topology of the modeled α-1,3-GalT resembles those of GnT I and SpsA with the secondary structural elements similarly arranged in space. The following amino acid residues have been identified to be part of the UDP docking pocket of α-1,3-GalT: Phe-134, Tyr-139, Ile-140, Val-136, Arg-194, Arg-202, Lys-209, Asp-173, His-218, Thr-137, Asp-225, Val-226, and Asp-227. The modeled catalytic domain has a core structure common to most of the known transferases (9-11). Moreover, amino acid residues that are involved in the UDP-Gal recognition and in the catalytic mechanism are homologous both in sequence and spatial relationship. As a consequence, the overall electrostatic property of the active site of the α-1,3-GalT is highly comparable with the UDP binding sites of GnTI and SpsA. Thus, the present analysis suggests that although the sequence homologies of SpsA, GnT I and α-1,3-GalT are relatively low, they have a structurally conserved framework of about 100 residues that specifically recognize UDP.

Complex of α-1,3-GalT with UDP and UDP-Gal. – In the GnT I, SpsA, and β4Gal T1 structures (9-11), the above-described architecture of the secondary structure elements specifically recognizes UDP. In these X-ray structures, a conserved aspartate (Asp39 in SpsA and Asp144 in GnT I) generally interacts though the hydrogen bond interaction with the carbonyl at the 4th position of the uracil ring. The carbonyl at the 2nd position of the uracil favors charge interactions with the conserved His residue that resides at the bottom of the UDP pocket. The ribose ring packs with the conserved hydrophobic residue (Thr-9 in SpsA and Ile-113 in GnT I) that is located at the bottom of the pocket. In the model of α-1,3-GalT, the metal binding site is located at one of the β-strands that contains the conserved DVD (Asp-225, Val-226 and Asp227) motif. These conserved residues are assumed to be located in the vicinity of the pyrophosphate-binding region. The C-terminal portion of the model has a confined groove, which has a stretch of charged residues. The docking studies described below suggest that this region can specifically recognize inhibitors, which are designed based on the acceptor substrate model (19).

Simulation of the α-1,3-GalT-UDP complexes, using an automated docking procedure led to several complex structures that represent different binding modes of UDP, which were clustered to nine groups. Analysis of results revealed that in about 80% of the docking calculations, the UDP binds at the well-defined pocket located at the DVD motif. The low energy docking modes of UDP to the α-1,3-GalT are shown in Figure 3. The α-1,3-GalT structure is presented in ribbon form and the amino acid residues that directly interact with UDP are labeled. Five top ranking clusters are characterized in Table 2 together with the computed binding energy and the estimated inhibition constant. Possible intermolecular contacts in the lowest energy complex are listed in Table 1. In the top three clusters, UDP binds in the deep pocket generally in a similar conformation. This is illustrated in Figure 3, where the preferred binding mode is shown as a thick blue tube. Three hydrogen bonds that are possible between the uracil and α-1,3-GalT characterize this binding mode. These are (1) the amide hydrogen of uracil in position 3 and OD1 of Asp-168, (2) the carbonyl oxygen of uracil in position 4 and the side chain of Lys-204, and (3) the carbonyl oxygen of uracil in position 2 and the amide hydrogen of the His-213 side chain. The hydroxyl groups at the 2 and 3 positions of the

ribose ring forms three hydrogen bonds with the Asp-225 side chain oxygens. The pyrophosphate oxygens interact with the Asp-227 side chain through the metal ion. Apart from these hydrogen bond interactions many favorable hydrophobic interactions are possible between the uridine and the protein. It is clear from Table 1 that the bound UDP generally favors interactions with conserved amino acid residues of the enzyme. However, some of the residues that do not interact directly with UDP but lie in the close vicinity of the UDP docked region are Tyr-139, Ile-140, Val-136, Arg-194, Asp-197, Ile-198, Arg-202, Lys-204, His209 and His-213. It is noteworthy that some of these residues such as Tyr139, Asp-197 are conserved across various species (8). It is possible that these active site side chains may be involved in direct binding interactions with UDP.

The lowest energy cluster consists of about 30% of all the docking runs. The analysis of the other low energy clusters that represent about 70% of docked structures clearly shows that many of the docking modes were very close to the lowest energy-binding mode. However, small variations in the nature of local interactions between the pyrophosphate part and the enzyme were observed. It can be seen from Figure 3 that the 5 and 6 positions of the uracil ring are exposed to the solvent and the remaining positions of the uracil fragment are in contact with the protein.

The structure of the UDP-Gal complex with α-1,3-GalT has been generated using the approach described above. Figure 4 shows the low energy binding modes of this complex. The comparison of the α-1,3-GalT complexes with UDP and UDP-Gal reveals that the uridine portion of the UDP-Gal assumes a similar binding orientation as in the case of the α-1,3-GalT-UDP complex. These results suggest that the addition of the galactopyranose residue to UDP does not alter the binding mode of the uridine, which is tightly bound in the active site. On the contrary, the pyrophosphate is more flexible and its conformation alters upon addition of this monosaccharide unit to the UDP. These data indicate that the design of an inhibitor based on the docking sites of pyrophosphate and donor sugar group fragments of UDP-Gal should consider the possible conformational flexibility of the pyrophosphate group and the corresponding diversity associated with binding interactions.

In the crystal structure of the complex of SpsA with UDP, the UDP is bound at the active site of the enzyme (8). The uracil ring of the bound UDP is placed into the cavity where its carbonyl and amide hydrogens form two hydrogen bonds with side-chains of Arg-71 and Asp-39, respectively. Apart from these hydrogen bond interactions, a favorable stacking interaction between the uracil ring and side chain of Tyr-11 is possible. A strong hydrogen bond interaction is possible between the hydroxyl of ribose in the position 3 and the side chain oxygen of Asp-99. The pyrophosphate conformation is confined to a particular orientation due to the favorable charge interactions with the bound metal ion. Unligil et al (10) has solved a structure of GnT I complexed with UDP-GlcNAc at 1.5 Å resolution. In this crystal structure of the GnT I complex, the uracil ring favors a similar interaction, as observed in the SpsA complex, with the nucleotide binding domain residues consisting of a Lys and an Asp. The ribose portions of the UDP bind into the hydrophobic rich region of the GnT I and thereby gains a stacking energy. Thus, these two structures possess a clear structural and sequence similarity at the UDP binding pocket. However, overall there is no sequence homology between the two proteins. The bound UDP conformation is very similar in these structural complexes. These data suggest that amino acid conservation at the UDP binding pocket is important for the precise recognition of UDP ligands. The homology model of α-1,3-GalT contains these critical amino acids at the identified pocket of the enzyme (Figures 2 and 3). The top ranking docked complexes are in agreement with reported X-ray structures of glycosyltransferases (7, 9, and 11). This suggests that a part of the substrate binding pocket in glycosyltrasferases is specifically tailored to bind UDP. It is evident from the computed docking models that the binding modes of UDP

generally favor a standard type of interaction with the enzyme. In the predicted low energy complexes of UDP and UDP-Gal with α-1,3-GalT, the DVD motif of the enzyme interacts with pyrophosphate through the modeled metal cation.

Binding mode of an inhibitor to α-1,3-GalT

Recently, an inhibitor based on the acceptor of α-1,3-GalT has been designed (19). This compound has a disaccharide linked to a bromine substituted naphthamide ring. It has been shown that the removal of the terminal sugar unit in this inhibitor does not inhibit α-1,3-GalT, but instead inhibits β-1,4-GalT. Thus, the determination of the binding mode of this inhibitor to α-1,3-GalT might provide a stereochemical explanation for the observed binding affinities. Using the above described docking procedure, this synthetic inhibitor was docked to the surface of α-1,3-GalT. Docking simulations produced two distinct favorable regions for this molecule located in the active site of the enzyme. In the one, the inhibitor occupies the UDP binding site. Generally, in this low energy binding mode the inhibitor is placed well in the uridine pocket. The second largest cluster of conformations is located at the acceptor site. Figure 5 shows the computed binding mode of the inhibitor at the acceptor-binding region of the protein. In this binding mode, the terminal saccharide binds close to the Asp-227 side chain and the bulky aromatic group of the inhibitor interacts with the side chain of of Ile-283. The bromide atom is located close to the side chain of Asp-227 and the naphthamide ring is placed on the top of Met-224 side chain. It can be seen that the inhibitor not only occupies the acceptor-binding region of the protein but also has considerable interactions at the donor site of the enzyme. Thus, these predicted binding modes of inhibitor could explain its inhibitory activity.

Figures 6 to 9 also show models of α-1,3-GalT and ligand binding domains of the enzyme.

Conclusions

Using a combination of homology modeling and molecular docking approaches, the α-1,3-GalT structure and its complexes with UDP, UDP-Gal, and a synthetic inhibitor have been modeled. The predicted N-terminal domain of the of the α-1,3-GalT has about 100 residues that start at Gln-125 and end at Gln-131. The overall secondary structure arrangements, amino acid properties, spatial arrangement of critical amino acid residues and size of this domain are highly comparable with other GnT structures. The predicted pocket on this domain surface of α-1,3-GalT specifically recognizes UDP in a unique binding mode. Structural analysis and comparative studies of the modeled binding site with the GnT I and SpsA structures suggested the high degree of similarity at the UDP binding pocket. This implies a possible structural homology in glycosyltransferases in spite of their low sequence identity and homology. Thus the modeled bovine structure of α-1,3-GalT provides a framework to better understand the functional and structural similarities between galactosyltransferases.

While the present invention has been described with reference to what are presently considered to be the preferred examples, it is to be understood that the invention is not limited to the disclosed examples. To the contrary, the invention is intended to cover various modifications and equivalent arrangements included within the spirit and scope of the appended claims.

All publications, patents and patent applications are herein incorporated by reference in their entirety to the same extent as if each individual publication, patent or patent application was specifically and individually indicated to be incorporated by reference in its entirety.

References

1. Varki A. Biological roles of oligosaccharides: all of the theories are correct. Glycobiology 1993; 3: 97-130.
2. Montreuil J, Vliegenthart JFG, Schachter H. Glycoproteins and Disease; Neuberger A. and van Deenen LLM, editors. Amsterdam: Elsevier; 1995. Vol. 30.
3. Paulson JC, Colley KJ. Glycosyltransferases – structure, location, and control of cell type-specific glycosylation. J Biol Chem 1989; 264: 17614-17618.
4. Campbell JA, Davies G J, Bulone V, Henrissat B. A classification of nucleotide-diphospho-sugar glycosyltransferases based on amino acid sequence similarities. Biochem J 1997; 326: 929-942.
5. Chen X, Andreana PR, Wang PG. Carbohydrates in transplantation. Curr Opinion Chem Biol 1999; 3: 650-658.
6. Galili U. 1992. In Bona C, Kaushik AK. editors, Molecular Immunobiology of Self-Reactivity. Marcel Dekker, Inc., New York, NY, pp. 355-373.
7. Vrielink A, Ruger W, Driessen HPC, Freemont PS. Crystal structure of the DNA modifying enzyme β-glucosyltransferase in the presence and absence of the substrate uridine diphosphoglucose. EMBO J 1994; 13: 3413-3422.
8. Imberty A, Monier C, Bettler E, Morera S, Freemont P, Sippl M, Flockner H, Ruger W, Breton C. Fold recognition study of α3-galactosyltransferase and molecular modeling of the nucleotide sugar-binding domain. Glycobiology 1999; 9: 713-722.
9. Charnock SJ, Davies GJ. Structure of the nucleotide-diphospho-sugar transferase, SpsA from Bacillus subtilis, in native and nucleotide-complexed forms. Biochemistry 1999; 38: 6380-6385.
10. Gastinel LN, Cambillau C, Bourne Y. Crystal structures of the bovine β4galactosyltransferase catalytic domain and its complex with uridine diphosphogalactose. EMBO J 1999; 18: 3546-3557.
11. Unligil UM, Zhou S, Yuwaraj S, Sarkar M, Schachter H, Rini JM. X-ray crystal Structure of rabbit N-acetylglucosaminyltransferase I: catalytic mechanism and a new protein superfamily. EMBO J 2000; 20: 5269-5280.
12. Zemla A, Venclovas C, Moult J, Fidelis K. Processing and analysis of CASP3 protein structure predictions. Proteins Suppl 1999; 3: 222-9;
13. http://www.ncbi.nlm.nih.gov:80/entrez
14. Rice D, Fischer D, Weiss R, Eisendberg D. (1997). Fold assignments for amino acid sequences of the CASP2 experiment. Proteins Suppl 1: 113-22; http://fold.doe-mci.ucla.edu.
15. HOMOLOGY, User Guide, 1997, San Diego MSI, 1997.
16. MODELER, User Guide, 1997, San Diego MSI, 1997.
17. Insight II, User Guide, 1997, San Diego MSI, 1997.
18. Needlman SB, Wunsch CD. A general method applicable to the search for similarities in the amino acid sequence of two proteins. J Mol Biol 1970; 48: 443-453.
19. Chung S, Takayama S, Wong C. Acceptor substrate-based selective inhibition of galactosyltransferases. Bioorg Med Chem 1998; 8: 3359-3364.
20. Morris GM, Goodsell DS, Hallidy RS, Huey R, Hart WE, Belew RK, Olson A.J. Automated Docking Using a Lamarckian Genetic Algorithm and and Empirical Binding Free Energy Function. J Comput Chem 1998; 19: 1639-1662.

21. Hagen FK, Hazes B, Raffo R, deSa D, Tabak LA. Structure-function analysis of the UDP-N-acetyl-d-galactosamine: polypeptide N-acetylgalactosaminyltransferase. J Biol Chem 1999; 274: 6797-6803.

22. Ramkrishnan C, Ramachandran GN. Stereochemical criteria for polypetide and protein chain conformations. II. Allowed conformations for a pair of peptide unit. Biophys J 1965; 5: 909-933.

5

Table 1

Atomic Interactions between GalT and UDP

Atomic Interaction	Atomic Contact on UDP	Atomic Contact on GalT	Distance Between Atomic Contacts on GalT and UDP	Nature of Interaction
1	Uracil NH	Asp-168 OD1	2.1 ± 0.5	HB
2	Uracil O1	Lys-204 HZ1	3.0 ± 0.5	HB
3	Uracil 02	His-213 NE2	2.7 ± 0.5	HB
4	Uracil Ring	Phe 134 Ring	4.2 ± 0.5	HP
5	Ribose OH2	Asp-225 OD2	2.2 ± 0.5	HB
6	Ribose OH3	Asp –225 OD2	2.5 ± 0.5	HB
7	Ribose ring	Leu 131	4.1 ± 0.5	HP
8	Ribose Ring	Ile-210	4.0 ± 0.5	HP
9	O1a (Diphosphate)	Asp-225 OD2(Mn)	4.6 ± 0.5	MM
10	O1a (diphosphate)	Asp-227 OD2(Mn)	4.5 ± 0.5	MM
11	O2b (diphosphate)	Asp-227 OD2(Mn)	5.1 ± 0.5	MM

HB: hydrogen bond interaction

MM: metal mediated interaction

HP: hydrophobic interaction

Table 2

Characterization of the Top Five Binding Modes of UDP to the α-1,3-GalT

Cluster Rank	Number of Conformers in Cluster	Computed Free energy in Kcal/mol	Calculated inhibition constant in μM
1	30	-8.72	0.40
2	24	-8.42	0.60
3	16	-8.18	1.00
4	6	-7.63	2.50
5	7	-7.54	2.90

Table 3

alphagt

PHD prediction:

```
                 ....,....1....,....2....,....3....,....4....,....5....,....6
         AA      |MNVKGKVILSMLVVSTVIVVFWEYIHSPEGSLPWINPSRNPEVGGSSIQKGWWLPRWFNN|
         PHD sec |   EEEEEEEEEEEEEEEEEEEEEEE      EEEEEE                    |
         Rel sec |994125899999887788999988548877468897135531165644354433355657|
detail:
         prH sec |000000000000000000000000000000000000000000000000122111221112111|
         prE sec |003556899989888888999888731011278887432234422112222222311121|
         prL sec |996432100000111111000011268877621001466754476765566555566667|
subset:  SUB sec |LL...EEEEEEEEEEEEEEEEEEE.LLLL.EEEEE..LL...LLL...L.....LLLLL|

ACCESSIBILITY
3st:     P_3 acc |eebebebbbbbbbbbbbbbbbbbbebeebbbbbbbbbb bbebbeebb eebbbe bbee|
10st:    PHD acc |970706000000000000000020609700000000050070067005772006500077|
         Rel acc |551641779865576498879500310241445682221214220301133011110243|
subset:  SUB acc |ee.eb.bbbbbbbbbbbbbbbb......e.bbbbb......e.................e.|
                 ....,....7....,....8....,....9....,....10...,....11...,....12
         AA      |G...YHEEDGDINEEKEQRNEDE.SKLKLSDWFNPFKRPEVVTMTKWKAPVVWEGTYNRA|
         PHD sec |                                        EEEEE    EEEEE    HH|
         Rel sec |863322265433522467767778887544555989999268886267713661255527|
detail:
         prH sec |111111112233234211121110000112111000000000000000000000001257|
         prE sec |013333310000000000000000122111100000047888741115677432211C|
         prL sec |865554566655655677777778887665666989899521011578843124566631|
subset:  SUB sec |LL.....LL...L...LLLLLLLLLLLL..LLLLLLLLL.EEEEE.LLL..EE..LLL.H|

ACCESSIBILITY
3st:     P_3 acc |bbbbbbeeeecbeeeeeeeeeeeeeebebbebb eee eebbbbbbebebebbbebb  bb|
10st:    PHD acc |000006777707767776777677060070057995870000062606000700450O|
         Rel acc |210200133340351444144431450220401144513545241101313434201114|
subset:  SUB acc |..........e..e.eee.eee..ee....e...eee..ebb.b.......b.e.....b|
                 ....,....13...,....14....,....15...,....16....,....17...,....18
         AA      |VLDNYYAKQKITVGLTVFAVGRYIEHYLEEFLTSANKHFMVGHPVIFYINVDDVSRMPLI|
         PHD sec |HHHHHHHHHHEEEE EEEEEEHHHHHHHHHHHHHHHHHHEEEEEEEEEEEEEE      EE|
         Rel sec |899995652147405867522599999999999853215544459999997177788246|
detail:
         prH sec |889986764310000000025799999999999865432111000000000000100000|
         prE sec |000000012367646878740000000000000001466666689999975100003G7|
         prL sec |000002222221242111133200000000000123321122220000001488888522|
subset:  SUB sec |HHHHHHHH...E..EEEEE..HHHHHHHHHHHHHH...EE...EEEEEEEE.LLLLL..E|

ACCESSIBILITY
3st:     P_3 acc |bbee bbeeebbbbbbbbbbbebbebbbeebbebbebbbbbbbbebbbbbbbe bbebbbb|
10st:    PHD acc |007740077700000000006006000760060070000000600000007500600O0|
         Rel acc |554410143530507473781228103651542043025452228894874301213135|
subset:  SUB acc |bbee...e.e..b.bbb.bb...b...be.bb..b...bbb...bbbbbbb........b|
                 ....,....19...,....20....,....21...,....22...,....23...,....24
         AA      |ELGPLRSFKVFKIKPEKRWQDISMMRMKTIGEHIVARIQHEVDFLFCMDVDQVFQDKPGV|
         PHD sec |EE      EEEEEEE   HHHHHHHHHHHHHHHHHHHHHHHHHEEEEEEEEEEE      |
         Rel sec |548785148888615434587999999996899988764223578998434112157552|
detail:
         prH sec |000000100000001236688888899987889988775422110000011232110100|
         prE sec |761112468888742000000000000000000000011224567888865532232112З|
         prL sec |238886431011146653211000000002100001112322210001232344467665|
subset:  SUB sec |E.LLLL..EEEEE.L...HHHHHHHHHHHHHHHHHHHHH....EEEEEE.......LLLL.|
```

5

```
ACCESSIBILITY
3st:     P_3 acc |ebbe  bbebbebeeeeebeebbbb bebbbebbbbbbebebbbbbbbebe bbee bbb
10st:    PHD acc |600745006007067776077000050600070000006060000000606500675006
         Rel acc |130302122454423463133542327216342943062115055863041223131215
subset:  SUB acc |.........bbeb..ee....bb...b..b.e.bb..b...b.bbbb..b.........b
                  ....,....,25...,....26...,....27...,....28...,....29.....,....3
         AA      |ETLGESVAQLQAWWYKADPNDFTYERRKESAAYIPFGEGDFYYHAAIFGGTPTQVLNITQ
         PHD sec |EE HHHHHHHHHHHHH    HHHHH        EE      EEEEEEE    HHHHHHHHH
         Rel sec |231356899887643138831133211122342214767456787613897458888885
detail:
         prH sec |013577889887765320134455433433321110000111000111001668888885
         prE sec |553000000000123220000111221000124542111267787742000000000006
         prL sec |333321100001111358864333344455553346777621101135898321111100
subset:  SUB sec |....HHHHHHHHH....LL.................LLL.EEEEEE..LLL.HHHHHHHH

ACCESSIBILITY
3st:     P_3 acc |ebbbebbbeb bbbbeb eeebe e eeebbbbbeeeeb bbbbbbbbee beebbebbe
10st:    PHD acc |600070006050000705777065756760000066970500000000995066006006
         Rel acc |235043452513030401464221512712241510340151249632531011711512
subset:  SUB acc |..b.e.bb.b.....e..eee...e..e...b.b...e..b..bbb..e.....b..b..
                  ....,....,31...,....,32.....,33...,....34...,....35...,....3
         AA      |ECFKGILKDKKNDIEAQWHDESHLNKYFLLNKPTKILSPEYCWDYH.IGLPADIKLVKMS
         PHD sec |HHHHHHHHHH    EEE      HHHHEEEEE   EE       HHHHH    HHH EEEE
         Rel sec |999999754246621332352111134555388513174220234432452111216788
detail:
         prH sec |999999766521121111223444452222100000001334455553213443221100
         prE sec |000000111000034553200001115666510245412111212111111112337788
         prL sec |000000112467744325565544421101288643586444332224564443431000
subset:  SUB sec |HHHHHHHH...LL......L.......EEE.LLL...L...........L......EEEE

ACCESSIBILITY
3st:     P_3 acc |ebbebbbeeeeeebebbb eee b ebbbbeeeeebbbeebbbebbbbbbebbbebbebb|
10st:    PHD acc |700700067677607000577750570000777670007720070000006000600600|
         Rel acc |464512214154025700133323140340463150134515130154021204236241|
subset:  SUB acc |ebbe....e.ee..eb.........e..b.ee..e...ee.b....bb.....b..b.b.|
                  ....,....37...,....38...,....39...,....40...,....41...,....42
         AA      |WQTKEYNVVRNNV|
         PHD sec |EE          |
         Rel sec |6323432215799|
detail:
         prH sec |0122232221100|
         prE sec |7531112231000|
         prL sec |1345654446799|
subset:  SUB sec |E........LLLL|

ACCESSIBILITY
3st:     P_3 acc |be ee ebbeeee|
10st:    PHD acc |0657736006799|
         Rel acc |1206411242333|
subset:  SUB acc |...ee...b....|
```

TABLE 4

ATOM	1	N	GLN	129	-4.878	33.589	36.449
ATOM	2	HN1	GLN	129	-4.249	34.321	36.811
ATOM	3	HN2	GLN	129	-4.600	33.343	35.488
ATOM	4	CA	GLN	129	-4.790	32.431	37.282
ATOM	5	HA	GLN	129	-5.554	32.501	38.056
ATOM	6	CB	GLN	129	-5.062	31.113	36.543
ATOM	7	HB1	GLN	129	-4.999	30.257	37.215
ATOM	8	HB2	GLN	129	-4.343	30.949	35.740
ATOM	9	CG	GLN	129	-6.456	31.098	35.916
ATOM	10	HG1	GLN	129	-6.680	30.069	35.633
ATOM	11	HG2	GLN	129	-6.432	31.752	35.044
ATOM	12	CD	GLN	129	-7.437	31.609	36.963
ATOM	13	OE1	GLN	129	-7.663	30.975	37.993
ATOM	14	NE2	GLN	129	-8.032	32.803	36.697
ATOM	15	HE2	GLN	129	-7.816	33.303	35.822
ATOM	16	HE2	GLN	129	-8.700	33.208	37.369
ATOM	17	C	GLN	129	-3.430	32.389	37.898
ATOM	18	O	GLN	129	-2.451	32.890	37.347
ATOM	19	N	LYS	130	-3.379	31.794	39.100
ATOM	20	HN	LYS	130	-4.252	31.369	39.444
ATOM	21	CA	LYS	130	-2.232	31.691	39.951
ATOM	22	HA	LYS	130	-1.740	32.653	40.094
ATOM	23	CB	LYS	130	-2.600	31.151	41.342
ATOM	24	HB1	LYS	130	-1.751	31.071	42.021
ATOM	25	HB2	LYS	130	-3.039	30.153	41.325
ATOM	26	CG	LYS	130	-3.620	32.014	42.090
ATOM	27	HG1	LYS	130	-3.849	31.529	43.039
ATOM	28	HG2	LYS	130	-4.516	32.095	41.475
ATOM	29	CD	LYS	130	-3.137	33.432	42.397
ATOM	30	HD1	LYS	130	-3.945	34.135	42.598
ATOM	31	HD2	LYS	130	-2.565	33.884	41.586
ATOM	32	CE	LYS	130	-2.224	33.518	43.622
ATOM	33	HE1	LYS	130	-2.626	32.907	44.430
ATOM	34	HE2	LYS	130	-2.152	34.551	43.962
ATOM	35	NZ	LYS	130	-0.869	33.030	43.278
ATOM	36	HZ1	LYS	130	-0.261	33.091	44.107
ATOM	37	HZ2	LYS	130	-0.925	32.050	42.965
ATOM	38	HZ3	LYS	130	-0.477	33.609	42.521
ATOM	39	C	LYS	130	-1.201	30.759	39.397
ATOM	40	O	LYS	130	-0.005	30.974	39.587
ATOM	41	N	ILE	131	-1.619	29.692	38.694
ATOM	42	HN	ILE	131	-2.598	29.601	38.388
ATOM	43	CA	ILE	131	-0.643	28.688	38.389
ATOM	44	HA	ILE	131	0.116	28.575	39.162
ATOM	45	CB	ILE	131	-1.212	27.300	38.320
ATOM	46	HB	ILE	131	-1.745	27.101	39.250
ATOM	47	CG2	ILE	131	-2.172	27.231	37.122
ATOM	48	HG2	ILE	131	-2.597	26.230	37.054
ATOM	49	HG2	ILE	131	-2.973	27.957	37.257
ATOM	50	HG2	ILE	131	-1.627	27.458	36.206
ATOM	51	CG1	ILE	131	-0.082	26.256	38.292
ATOM	52	HG1	ILE	131	0.695	26.441	39.033
ATOM	53	HG1	ILE	131	0.438	26.208	37.335
ATOM	54	CD1	ILE	131	-0.566	24.832	38.560
ATOM	55	HD1	ILE	131	0.281	24.147	38.526
ATOM	56	HD1	ILE	131	-1.030	24.785	39.545
ATOM	57	HD1	ILE	131	-1.294	24.546	37.802
ATOM	58	C	ILE	131	0.108	28.958	37.133
ATOM	59	O	ILE	131	-0.444	29.257	36.075
ATOM	60	N	THR	132	1.443	28.868	37.270
ATOM	61	HN	THR	132	1.826	28.697	38.211
ATOM	62	CA	THR	132	2.359	28.998	36.182
ATOM	63	HA	THR	132	1.727	29.134	35.304
ATOM	64	CB	THR	132	3.354	30.109	36.364

ATOM	65	HB	THR	132	2.812	31.041	36.525
ATOM	66	OG1	THR	132	4.162	30.248	35.205
ATOM	67	HG1	THR	132	4.271	31.247	34.980
ATOM	68	CG2	THR	132	4.232	29.788	37.584
ATOM	69	HG2	THR	132	4.960	30.586	37.729
ATOM	70	HG2	THR	132	3.606	29.703	38.472
ATOM	71	HG2	THR	132	4.755	28.846	37.418
ATOM	72	C	THR	132	3.127	27.718	36.179
ATOM	73	O	THR	132	3.437	27.174	37.238
ATOM	74	N	VAL	133	3.424	27.170	34.989
ATOM	75	HN	VAL	133	3.112	27.603	34.109
ATOM	76	CA	VAL	133	4.191	25.963	34.990
ATOM	77	HA	VAL	133	4.260	25.629	36.026
ATOM	78	CB	VAL	133	3.579	24.853	34.180
ATOM	79	HB	VAL	133	3.467	25.193	33.150
ATOM	80	CG1	VAL	133	4.509	23.630	34.237
ATOM	81	HG1	VAL	133	4.077	22.817	33.653
ATOM	82	HG1	VAL	133	5.483	23.894	33.826
ATOM	83	HG1	VAL	133	4.627	23.310	35.272
ATOM	84	CG2	VAL	133	2.171	24.570	34.735
ATOM	85	HG2	VAL	133	1.708	23.768	34.162
ATOM	86	HG2	VAL	133	2.245	24.273	35.781
ATOM	87	HG2	VAL	133	1.561	25.471	34.657
ATOM	88	C	VAL	133	5.534	26.296	34.425
ATOM	89	O	VAL	133	5.641	26.933	33.380
ATOM	90	N	GLY	134	6.606	25.880	35.122
ATOM	91	HN	GLY	134	6.480	25.331	35.984
ATOM	92	CA	GLY	134	7.924	26.201	34.664
ATOM	93	HA1	GLY	134	8.466	26.642	35.501
ATOM	94	HA2	GLY	134	7.825	26.909	33.841
ATOM	95	C	GLY	134	8.565	24.937	34.214
ATOM	96	O	GLY	134	8.578	23.936	34.928
ATOM	97	N	LEU	135	9.135	24.962	33.001
ATOM	98	HN	LEU	135	9.132	25.827	32.441
ATOM	99	CA	LEU	135	9.745	23.777	32.495
ATOM	100	HA	LEU	135	9.529	22.955	33.178
ATOM	101	CB	LEU	135	9.288	23.401	31.082
ATOM	102	HB1	LEU	135	9.436	24.224	30.383
ATOM	103	HB2	LEU	135	8.230	23.142	31.061
ATOM	104	CG	LEU	135	10.068	22.194	30.542
ATOM	105	HG	LEU	135	11.124	22.437	30.425
ATOM	106	CD2	LEU	135	9.638	21.839	29.113
ATOM	107	HD2	LEU	135	10.211	20.980	28.764
ATOM	108	HD2	LEU	135	8.576	21.595	29.102
ATOM	109	HD2	LEU	135	9.822	22.689	28.456
ATOM	110	CD1	LEU	135	9.956	21.005	31.498
ATOM	111	HD1	LEU	135	10.516	20.161	31.095
ATOM	112	HD1	LEU	135	10.364	21.280	32.470
ATOM	113	HD1	LEU	135	8.908	20.725	31.610
ATOM	114	C	LEU	135	11.215	23.999	32.405
ATOM	115	O	LEU	135	11.682	25.098	32.119
ATOM	116	N	THR	136	11.994	22.945	32.698
ATOM	117	HN	THR	136	11.563	22.078	33.052
ATOM	118	CA	THR	136	13.413	23.007	32.527
ATOM	119	HA	THR	136	13.609	24.037	32.229
ATOM	120	CB	THR	136	14.187	22.632	33.762
ATOM	121	HB	THR	136	15.253	22.703	33.546
ATOM	122	OG1	THR	136	13.894	21.296	34.144
ATOM	123	HG1	THR	136	12.992	21.271	34.641
ATOM	124	CG2	THR	136	13.814	23.602	34.899
ATOM	125	HG2	THR	136	14.370	23.339	35.799
ATOM	126	HG2	THR	136	14.063	24.621	34.604
ATOM	127	HG2	THR	136	12.745	23.534	35.100
ATOM	128	C	THR	136	13.710	22.003	31.462
ATOM	129	O	THR	136	13.227	20.872	31.523
ATOM	130	N	VAL	137	14.487	22.397	30.431
ATOM	131	HN	VAL	137	14.898	23.340	30.399
ATOM	132	CA	VAL	137	14.718	21.447	29.381

ATOM	133	HA	VAL	137	14.363	20.462	29.683
ATOM	134	CB	VAL	137	14.014	21.789	28.099
ATOM	135	HB	VAL	137	14.297	21.056	27.343
ATOM	136	CG1	VAL	137	12.497	21.745	28.349
ATOM	137	HG1	VAL	137	11.969	21.991	27.427
ATOM	138	HG1	VAL	137	12.210	20.745	28.675
ATOM	139	HG1	VAL	137	12.234	22.468	29.121
ATOM	140	CG2	VAL	137	14.536	23.149	27.604
ATOM	141	HG2	VAL	137	14.035	23.413	26.672
ATOM	142	HG2	VAL	137	14.332	23.912	28.355
ATOM	143	HG2	VAL	137	15.610	23.086	27.433
ATOM	144	C	VAL	137	16.179	21.363	29.078
ATOM	145	O	VAL	137	16.898	22.362	29.101
ATOM	146	N	PHE	138	16.663	20.128	28.828
ATOM	147	HN	PHE	138	16.051	19.306	28.928
ATOM	148	CA	PHE	138	18.025	19.961	28.425
ATOM	149	HA	PHE	138	18.327	20.795	27.792
ATOM	150	CB	PHE	138	19.021	19.919	29.599
ATOM	151	HB1	PHE	138	18.676	19.145	30.284
ATOM	152	HB2	PHE	138	19.009	20.904	30.064
ATOM	153	CG	PHE	138	20.360	19.595	29.027
ATOM	154	CD1	PHE	138	21.167	20.575	28.499
ATOM	155	HD1	PHE	138	20.829	21.612	28.499
ATOM	156	CD2	PHE	138	20.800	18.291	29.005
ATOM	157	HD2	PHE	138	20.164	17.504	29.412
ATOM	158	CE1	PHE	138	22.396	20.258	27.971
ATOM	159	HE1	PHE	138	23.030	21.043	27.558
ATOM	160	CE2	PHE	138	22.027	17.965	28.480
ATOM	161	HE2	PHE	138	22.363	16.928	28.473
ATOM	162	CZ	PHE	138	22.828	18.954	27.962
ATOM	163	HZ	PHE	138	23.804	18.704	27.545
ATOM	164	C	PHE	138	18.174	18.680	27.658
ATOM	165	O	PHE	138	18.069	17.587	28.211
ATOM	166	N	ALA	139	18.436	18.820	26.344
ATOM	167	HN	ALA	139	18.400	19.778	25.968
ATOM	168	CA	ALA	139	18.760	17.776	25.412
ATOM	169	HA	ALA	139	18.689	18.186	24.405
ATOM	170	CB	ALA	139	20.209	17.281	25.561
ATOM	171	HB1	ALA	139	20.401	16.492	24.833
ATOM	172	HB2	ALA	139	20.896	18.109	25.388
ATOM	173	HB3	ALA	139	20.358	16.889	26.567
ATOM	174	C	ALA	139	17.868	16.578	25.473
ATOM	175	O	ALA	139	18.359	15.456	25.348
ATOM	176	N	VAL	140	16.546	16.733	25.670
ATOM	177	HN	VAL	140	16.109	17.634	25.911
ATOM	178	CA	VAL	140	15.812	15.518	25.511
ATOM	179	HA	VAL	140	16.520	14.737	25.234
ATOM	180	CB	VAL	140	15.073	15.043	26.706
ATOM	181	HB	VAL	140	14.435	15.884	26.977
ATOM	182	CG1	VAL	140	14.311	13.812	26.211
ATOM	183	HG1	VAL	140	13.731	13.389	27.031
ATOM	184	HG1	VAL	140	13.639	14.101	25.402
ATOM	185	HG1	VAL	140	15.019	13.068	25.846
ATOM	186	CG2	VAL	140	16.062	14.743	27.846
ATOM	187	HG2	VAL	140	15.513	14.395	28.721
ATOM	188	HG2	VAL	140	16.763	13.972	27.526
ATOM	189	HG2	VAL	140	16.611	15.650	28.099
ATOM	190	C	VAL	140	14.803	15.735	24.437
ATOM	191	O	VAL	140	13.632	16.009	24.704
ATOM	192	N	GLY	141	15.244	15.558	23.183
ATOM	193	HN	GLY	141	16.215	15.244	23.042
ATOM	194	CA	GLY	141	14.425	15.788	22.033
ATOM	195	HA1	GLY	141	15.021	15.687	21.126
ATOM	196	HA2	GLY	141	14.004	16.793	22.071
ATOM	197	C	GLY	141	13.311	14.796	21.995
ATOM	198	O	GLY	141	12.214	15.108	21.538
ATOM	199	N	ARG	142	13.579	13.554	22.433
ATOM	200	HN	ARG	142	14.509	13.337	22.819

```
ATOM    201  CA  ARG  142      12.581  12.529  22.365
ATOM    202  HA  ARG  142      12.172  12.468  21.357
ATOM    203  CB  ARG  142      13.130  11.135  22.711
ATOM    204  HB1 ARG  142      12.356  10.368  22.729
ATOM    205  HB2 ARG  142      13.609  11.099  23.689
ATOM    206  CG  ARG  142      14.181  10.646  21.712
ATOM    207  HG1 ARG  142      15.085  11.239  21.848
ATOM    208  HG2 ARG  142      13.783  10.777  20.706
ATOM    209  CD  ARG  142      14.564   9.175  21.872
ATOM    210  HD1 ARG  142      13.654   8.593  21.725
ATOM    211  HD2 ARG  142      14.963   9.060  22.879
ATOM    212  NE  ARG  142      15.587   8.880  20.830
ATOM    213  HE  ARG  142      15.303   8.494  19.918
ATOM    214  CZ  ARG  142      16.903   9.124  21.093
ATOM    215  NH1 ARG  142      17.268   9.588  22.323
ATOM    216  HH1 ARG  142      18.260   9.775  22.529
ATOM    217  HH1 ARG  142      16.553   9.752  23.045
ATOM    218  NH2 ARG  142      17.848   8.912  20.131
ATOM    219  HH2 ARG  142      18.840   9.098  20.335
ATOM    220  HH2 ARG  142      17.568   8.566  19.202
ATOM    221  C   ARG  142      11.466  12.829  23.318
ATOM    222  O   ARG  142      10.302  12.577  23.012
ATOM    223  N   TYR  143      11.805  13.312  24.527
ATOM    224  HN  TYR  143      12.795  13.518  24.721
ATOM    225  CA  TYR  143      10.834  13.549  25.554
ATOM    226  HA  TYR  143      10.121  12.725  25.537
ATOM    227  CB  TYR  143      11.480  13.520  26.952
ATOM    228  HB1 TYR  143      10.718  13.833  27.665
ATOM    229  HB2 TYR  143      12.322  14.212  26.931
ATOM    230  CG  TYR  143      11.927  12.112  27.201
ATOM    231  CD1 TYR  143      11.169  11.057  26.750
ATOM    232  HD1 TYR  143      10.246  11.253  26.203
ATOM    233  CD2 TYR  143      13.049  11.829  27.950
ATOM    234  HD2 TYR  143      13.633  12.650  28.365
ATOM    235  CE1 TYR  143      11.559   9.758  26.979
ATOM    236  HE1 TYR  143      10.957   8.934  26.595
ATOM    237  CE2 TYR  143      13.447  10.536  28.185
ATOM    238  HE2 TYR  143      14.351  10.338  28.762
ATOM    239  CZ  TYR  143      12.704   9.493  27.691
ATOM    240  OH  TYR  143      13.106   8.161  27.926
ATOM    241  HH  TYR  143      12.350   7.654  28.408
ATOM    242  C   TYR  143      10.033  14.831  25.431
ATOM    243  O   TYR  143       8.809  14.823  25.543
ATOM    244  N   ILE  144      10.687  15.959  25.108
ATOM    245  HN  ILE  144      11.631  15.889  24.702
ATOM    246  CA  ILE  144      10.110  17.266  25.312
ATOM    247  HA  ILE  144       9.960  17.404  26.383
ATOM    248  CB  ILE  144      11.045  18.376  24.925
ATOM    249  HB  ILE  144      12.013  18.187  25.390
ATOM    250  CG2 ILE  144      11.176  18.388  23.394
ATOM    251  HG2 ILE  144      11.852  19.188  23.093
ATOM    252  HG2 ILE  144      11.572  17.431  23.055
ATOM    253  HG2 ILE  144      10.196  18.553  22.947
ATOM    254  CG1 ILE  144      10.563  19.706  25.525
ATOM    255  HG1 ILE  144      10.256  19.621  26.567
ATOM    256  HG1 ILE  144       9.705  20.127  25.002
ATOM    257  CD1 ILE  144      11.630  20.799  25.502
ATOM    258  HD1 ILE  144      11.225  21.711  25.940
ATOM    259  HD1 ILE  144      12.496  20.474  26.079
ATOM    260  HD1 ILE  144      11.931  20.992  24.473
ATOM    261  C   ILE  144       8.786  17.503  24.644
ATOM    262  O   ILE  144       7.929  18.176  25.216
ATOM    263  N   GLU  145       8.559  16.986  23.427
ATOM    264  HN  GLU  145       9.270  16.399  22.969
ATOM    265  CA  GLU  145       7.311  17.261  22.771
ATOM    266  HA  GLU  145       7.201  18.334  22.616
ATOM    267  CB  GLU  145       7.200  16.541  21.414
ATOM    268  HB1 GLU  145       7.489  15.499  21.553
```

	ATOM	269	HB2	GLU	145	7.869	17.033	20.708
	ATOM	270	CG	GLU	145	5.792	16.557	20.809
	ATOM	271	HG1	GLU	145	5.064	16.333	21.588
	ATOM	272	HG2	GLU	145	5.730	15.806	20.021
5	ATOM	273	CD	GLU	145	5.512	17.933	20.227
	ATOM	274	OE1	GLU	145	5.854	18.943	20.899
	ATOM	275	OE2	GLU	145	4.951	17.992	19.100
	ATOM	277	C	GLU	145	6.174	16.771	23.610
	ATOM	278	O	GLU	145	5.182	17.477	23.791
10	ATOM	279	N	HIS	146	6.300	15.550	24.158
	ATOM	280	HN	HIS	146	7.192	15.044	24.055
	ATOM	281	CA	HIS	146	5.227	14.935	24.880
	ATOM	282	HA	HIS	146	4.330	14.892	24.262
	ATOM	283	ND1	HIS	146	3.840	12.371	26.806
15	ATOM	284	HD1	HIS	146	4.262	12.665	27.699
	ATOM	285	CG	HIS	146	4.305	12.661	25.543
	ATOM	286	NE2	HIS	146	2.430	11.416	25.377
	ATOM	287	HE2	HIS	146	1.637	10.885	24.989
	ATOM	288	CD2	HIS	146	3.432	12.070	24.683
20	ATOM	289	HD2	HIS	146	3.511	12.106	23.596
	ATOM	290	CE1	HIS	146	2.717	11.624	26.648
	ATOM	291	HE1	HIS	146	2.122	11.240	27.477
	ATOM	292	CB	HIS	146	5.530	13.469	25.238
	ATOM	293	HB1	HIS	146	6.169	13.358	26.113
25	ATOM	294	HB2	HIS	146	6.040	12.924	24.443
	ATOM	295	C	HIS	146	4.915	15.719	26.121
	ATOM	296	O	HIS	146	3.747	15.885	26.466
	ATOM	297	N	TYR	147	5.938	16.225	26.842
	ATOM	298	HN	TYR	147	6.915	16.068	26.555
30	ATOM	299	CA	TYR	147	5.630	16.989	28.020
	ATOM	300	HA	TYR	147	5.026	16.397	28.707
	ATOM	301	CB	TYR	147	6.829	17.505	28.833
	ATOM	302	HB1	TYR	147	7.620	17.877	28.183
	ATOM	303	HB2	TYR	147	7.258	16.717	29.452
35	ATOM	304	CG	TYR	147	6.200	18.589	29.645
	ATOM	305	CD1	TYR	147	5.277	18.281	30.619
	ATOM	306	HD1	TYR	147	5.019	17.237	30.798
	ATOM	307	CD2	TYR	147	6.501	19.914	29.422
	ATOM	308	HD2	TYR	147	7.220	20.183	28.649
40	ATOM	309	CE1	TYR	147	4.673	19.260	31.369
	ATOM	310	HE1	TYR	147	3.953	18.993	32.142
	ATOM	311	CE2	TYR	147	5.901	20.902	30.169
	ATOM	312	HE2	TYR	147	6.154	21.947	29.991
	ATOM	313	CZ	TYR	147	4.982	20.576	31.140
45	ATOM	314	OH	TYR	147	4.365	21.589	31.905
	ATOM	315	HH	TYR	147	5.006	22.389	31.996
	ATOM	316	C	TYR	147	4.869	18.220	27.653
	ATOM	317	O	TYR	147	3.844	18.528	28.259
	ATOM	318	N	LEU	148	5.349	18.934	26.621
50	ATOM	319	HN	LEU	148	6.152	18.547	26.105
	ATOM	320	CA	LEU	148	4.823	20.193	26.187
	ATOM	321	HA	LEU	148	4.944	20.910	26.999
	ATOM	322	CB	LEU	148	5.608	20.637	24.935
	ATOM	323	HB1	LEU	148	5.473	19.864	24.178
55	ATOM	324	HB2	LEU	148	6.654	20.733	25.227
	ATOM	325	CG	LEU	148	5.229	21.964	24.264
	ATOM	326	HG	LEU	148	5.245	22.748	25.021
	ATOM	327	CD2	LEU	148	3.801	21.957	23.693
	ATOM	328	HD2	LEU	148	3.589	22.921	23.231
60	ATOM	329	HD2	LEU	148	3.712	21.169	22.945
	ATOM	330	HD2	LEU	148	3.088	21.776	24.497
	ATOM	331	CD1	LEU	148	6.255	22.258	23.160
	ATOM	332	HD1	LEU	148	6.002	23.199	22.670
	ATOM	333	HD1	LEU	148	7.250	22.333	23.599
65	ATOM	334	HD1	LEU	148	6.242	21.452	22.427
	ATOM	335	C	LEU	148	3.371	20.006	25.855
	ATOM	336	O	LEU	148	2.518	20.774	26.301
	ATOM	337	N	GLU	149	3.054	18.939	25.105

ATOM	338	HN	GLU	149	3.806	18.294	24.822
ATOM	339	CA	GLU	149	1.714	18.659	24.681
ATOM	340	HA	GLU	149	1.317	19.494	24.104
ATOM	341	CB	GLU	149	1.630	17.377	23.835
ATOM	342	HB1	GLU	149	2.205	16.546	24.243
ATOM	343	HB2	GLU	149	1.997	17.502	22.816
ATOM	344	CG	GLU	149	0.206	16.837	23.680
ATOM	345	HG1	GLU	149	-0.294	16.880	24.648
ATOM	346	HG2	GLU	149	0.256	15.805	23.331
ATOM	347	CD	GLU	149	-0.536	17.693	22.670
ATOM	348	OE1	GLU	149	0.137	18.476	21.949
ATOM	349	OE2	GLU	149	-1.789	17.573	22.607
ATOM	351	C	GLU	149	0.831	18.435	25.867
ATOM	352	O	GLU	149	-0.298	18.921	25.905
ATOM	353	N	GLU	150	1.332	17.710	26.881
ATOM	354	HN	GLU	150	2.321	17.422	26.863
ATOM	355	CA	GLU	150	0.502	17.335	27.988
ATOM	356	HA	GLU	150	-0.343	16.748	27.628
ATOM	357	CB	GLU	150	1.238	16.472	29.027
ATOM	358	HB1	GLU	150	1.833	17.063	29.723
ATOM	359	HB2	GLU	150	1.929	15.760	28.574
ATOM	360	CG	GLU	150	0.287	15.640	29.891
ATOM	361	HG1	GLU	150	-0.491	16.316	30.242
ATOM	362	HG2	GLU	150	0.880	15.237	30.713
ATOM	363	CD	GLU	150	-0.271	14.539	28.996
ATOM	364	OE1	GLU	150	-0.108	14.660	27.752
ATOM	365	OE2	GLU	150	-0.862	13.565	29.534
ATOM	367	C	GLU	150	-0.004	18.564	28.674
ATOM	368	O	GLU	150	-1.156	18.611	29.106
ATOM	369	N	PHE	151	0.859	19.584	28.821
ATOM	370	HN	PHE	151	1.819	19.495	28.458
ATOM	371	CA	PHE	151	0.458	20.792	29.476
ATOM	372	HA	PHE	151	0.018	20.581	30.450
ATOM	373	CB	PHE	151	1.638	21.741	29.732
ATOM	374	HB1	PHE	151	2.158	21.863	28.781
ATOM	375	HB2	PHE	151	2.269	21.267	30.483
ATOM	376	CG	PHE	151	1.063	23.023	30.218
ATOM	377	CD1	PHE	151	0.595	23.151	31.506
ATOM	378	HD1	PHE	151	0.642	22.301	32.187
ATOM	379	CD2	PHE	151	1.003	24.107	29.374
ATOM	380	HD2	PHE	151	1.375	24.016	28.353
ATOM	381	CE1	PHE	151	0.069	24.346	31.936
ATOM	382	HE1	PHE	151	-0.303	24.440	32.956
ATOM	383	CE2	PHE	151	0.479	25.302	29.800
ATOM	384	HE2	PHE	151	0.436	26.153	29.120
ATOM	385	CZ	PHE	151	0.010	25.422	31.084
ATOM	386	HZ	PHE	151	-0.406	26.369	31.427
ATOM	387	C	PHE	151	-0.559	21.534	28.661
ATOM	388	O	PHE	151	-1.590	21.955	29.184
ATOM	389	N	LEU	152	-0.310	21.684	27.346
ATOM	390	HN	LEU	152	0.509	21.214	26.936
ATOM	391	CA	LEU	152	-1.153	22.480	26.497
ATOM	392	HA	LEU	152	-1.211	23.501	26.874
ATOM	393	CB	LEU	152	-0.669	22.514	25.038
ATOM	394	HB1	LEU	152	-1.410	23.048	24.442
ATOM	395	HB2	LEU	152	-0.564	21.487	24.687
ATOM	396	CG	LEU	152	0.685	23.218	24.846
ATOM	397	HG	LEU	152	1.471	22.726	25.418
ATOM	398	CD2	LEU	152	0.667	24.632	25.454
ATOM	399	HD2	LEU	152	1.637	25.105	25.303
ATOM	400	HD2	LEU	152	-0.105	25.227	24.968
ATOM	401	HD2	LEU	152	0.458	24.566	26.521
ATOM	402	CD1	LEU	152	1.112	23.214	23.369
ATOM	403	HD1	LEU	152	2.072	23.719	23.267
ATOM	404	HD1	LEU	152	1.203	22.186	23.020
ATOM	405	HD1	LEU	152	0.363	23.735	22.772
ATOM	406	C	LEU	152	-2.534	21.905	26.455
ATOM	407	O	LEU	152	-3.523	22.634	26.528

	ATOM	408	N	THR	153	-2.624	20.568	26.352
	ATOM	409	HN	THR	153	-1.760	20.012	26.416
	ATOM	410	CA	THR	153	-3.865	19.882	26.156
	ATOM	411	HA	THR	153	-4.395	20.239	25.272
5	ATOM	412	CB	THR	153	-3.685	18.410	25.940
	ATOM	413	HB	THR	153	-2.933	18.254	25.167
	ATOM	414	OG1	THR	153	-4.907	17.832	25.510
	ATOM	415	HG1	THR	153	-5.654	18.539	25.547
	ATOM	416	CG2	THR	153	-3.223	17.764	27.257
10	ATOM	417	HG2	THR	153	-3.089	16.692	27.110
	ATOM	418	HG2	THR	153	-2.278	18.208	27.569
	ATOM	419	HG2	THR	153	-3.975	17.933	28.029
	ATOM	420	C	THR	153	-4.792	20.058	27.316
	ATOM	421	O	THR	153	-6.002	20.106	27.103
15	ATOM	422	N	SER	154	-4.245	20.151	28.550
	ATOM	423	HN	SER	154	-3.217	20.193	28.608
	ATOM	424	CA	SER	154	-4.981	20.196	29.791
	ATOM	425	HA	SER	154	-5.266	19.197	30.123
	ATOM	426	CB	SER	154	-4.167	20.786	30.955
20	ATOM	427	HB1	SER	154	-4.784	20.840	31.852
	ATOM	428	HB2	SER	154	-3.826	21.790	30.700
	ATOM	429	OG	SER	154	-3.037	19.970	31.221
	ATOM	430	HG	SER	154	-3.260	19.311	31.981
	ATOM	431	C	SER	154	-6.234	20.995	29.656
25	ATOM	432	O	SER	154	-6.230	22.221	29.738
	ATOM	433	N	ALA	155	-7.353	20.279	29.429
	ATOM	434	HN	ALA	155	-7.289	19.253	29.357
	ATOM	435	CA	ALA	155	-8.627	20.913	29.284
	ATOM	436	HA	ALA	155	-8.526	21.664	28.501
30	ATOM	437	CB	ALA	155	-9.751	19.926	28.929
	ATOM	438	HB1	ALA	155	-10.693	20.467	28.833
	ATOM	439	HB2	ALA	155	-9.518	19.433	27.986
	ATOM	440	HB3	ALA	155	-9.841	19.179	29.717
	ATOM	441	C	ALA	155	-8.963	21.528	30.594
35	ATOM	442	O	ALA	155	-9.412	22.669	30.649
	ATOM	443	N	ASN	156	-8.754	20.767	31.682
	ATOM	444	HN	ASN	156	-8.421	19.802	31.544
	ATOM	445	CA	ASN	156	-8.972	21.225	33.022
	ATOM	446	HA	ASN	156	-8.595	20.478	33.720
40	ATOM	447	CB	ASN	156	-8.254	22.544	33.350
	ATOM	448	HB1	ASN	156	-8.587	22.875	34.334
	ATOM	449	HB2	ASN	156	-8.520	23.274	32.586
	ATOM	450	CG	ASN	156	-6.756	22.281	33.348
	ATOM	451	OD1	ASN	156	-7.736	21.772	33.890
45	ATOM	452	ND2	ASN	156	-6.497	23.300	32.486
	ATOM	453	HD2	ASN	156	-5.527	23.497	32.199
	ATOM	454	HD2	ASN	156	-7.269	23.874	32.120
	ATOM	455	C	ASN	156	-10.432	21.427	33.237
	ATOM	456	O	ASN	156	-11.114	22.056	32.428
50	ATOM	457	N	LYS	157	-10.963	20.868	34.341
	ATOM	458	HN	LYS	157	-10.386	20.284	34.962
	ATOM	459	CA	LYS	157	-12.342	21.100	34.632
	ATOM	460	HA	LYS	157	-12.892	20.888	33.715
	ATOM	461	CB	LYS	157	-12.866	20.247	35.799
55	ATOM	462	HB1	LYS	157	-13.840	20.565	36.170
	ATOM	463	HB2	LYS	157	-12.214	20.255	36.673
	ATOM	464	CG	LYS	157	-13.039	18.769	35.448
	ATOM	465	HG1	LYS	157	-13.382	18.168	36.291
	ATOM	466	HG2	LYS	157	-12.115	18.301	35.109
60	ATOM	467	CD	LYS	157	-14.056	18.535	34.331
	ATOM	468	HD1	LYS	157	-14.141	17.489	34.036
	ATOM	469	HD2	LYS	157	-13.822	19.075	33.413
	ATOM	470	CE	LYS	157	-15.476	18.967	34.704
	ATOM	471	HE1	LYS	157	-15.486	20.021	34.983
65	ATOM	472	HE2	LYS	157	-15.839	18.377	35.545
	ATOM	473	NZ	LYS	157	-16.386	18.770	33.554
	ATOM	474	HZ1	LYS	157	-17.338	19.063	33.814
	ATOM	475	HZ2	LYS	157	-16.060	19.334	32.756

	ATOM	476	HZ3	LYS	157	-16.395	17.774	33.289
	ATOM	477	C	LYS	157	-12.453	22.529	35.040
	ATOM	478	O	LYS	157	-13.219	23.300	34.462
	ATOM	479	N	HIS	158	-11.653	22.918	36.051
5	ATOM	480	HN	HIS	158	-11.014	22.238	36.486
	ATOM	481	CA	HIS	158	-11.682	24.265	36.530
	ATOM	482	HA	HIS	158	-12.717	24.551	36.721
	ATOM	483	ND1	HIS	158	-12.504	24.615	39.778
	ATOM	484	HD1	HIS	158	-12.842	25.570	39.593
10	ATOM	485	CG	HIS	158	-11.570	23.919	39.043
	ATOM	486	NE2	HIS	158	-12.274	22.634	40.759
	ATOM	487	HE2	HIS	158	-12.386	21.843	41.409
	ATOM	488	CD2	HIS	158	-11.440	22.711	39.656
	ATOM	489	HD2	HIS	158	-10.774	21.914	39.325
15	ATOM	490	CE1	HIS	158	-12.892	23.800	40.792
	ATOM	491	HE1	HIS	158	-13.628	24.077	41.546
	ATOM	492	CB	HIS	158	-10.884	24.473	37.830
	ATOM	493	HB1	HIS	158	-10.697	25.522	38.059
	ATOM	494	HB2	HIS	158	-9.901	24.003	37.814
20	ATOM	495	C	HIS	158	-11.090	25.158	35.495
	ATOM	496	O	HIS	158	-11.707	26.144	35.098
	ATOM	497	N	PHE	159	-9.878	24.828	35.004
	ATOM	498	HN	PHE	159	-9.394	23.966	35.293
	ATOM	499	CA	PHE	159	-9.297	25.732	34.065
25	ATOM	500	HA	PHE	159	-9.603	26.738	34.353
	ATOM	501	CB	PHE	159	-7.764	25.681	34.055
	ATOM	502	HB1	PHE	159	-7.466	26.283	33.197
	ATOM	503	HB2	PHE	159	-7.517	24.624	33.951
	ATOM	504	CG	PHE	159	-7.349	26.262	35.362
30	ATOM	505	CD1	PHE	159	-7.253	25.470	36.482
	ATOM	506	HD1	PHE	159	-7.477	24.406	36.411
	ATOM	507	CD2	PHE	159	-7.082	27.607	35.474
	ATOM	508	HD2	PHE	159	-7.170	28.249	34.597
	ATOM	509	CE1	PHE	159	-6.877	26.007	37.691
35	ATOM	510	HE1	PHE	159	-6.798	25.367	38.570
	ATOM	511	CE2	PHE	159	-6.707	28.149	36.679
	ATOM	512	HE2	PHE	159	-6.492	29.215	36.753
	ATOM	513	CZ	PHE	159	-6.602	27.349	37.791
	ATOM	514	HZ	PHE	159	-6.301	27.777	38.748
40	ATOM	515	C	PHE	159	-9.814	25.368	32.728
	ATOM	516	O	PHE	159	-9.080	24.820	31.910
	ATOM	517	N	MET	160	-11.096	25.716	32.478
	ATOM	518	HN	MET	160	-11.620	26.224	33.205
	ATOM	519	CA	MET	160	-11.755	25.406	31.246
45	ATOM	520	HA	MET	160	-11.756	24.319	31.165
	ATOM	521	CB	MET	160	-13.167	26.013	31.157
	ATOM	522	HB1	MET	160	-13.568	25.796	30.168
	ATOM	523	HB2	MET	160	-13.085	27.088	31.314
	ATOM	524	CG	MET	160	-14.161	25.473	32.186
50	ATOM	525	HG1	MET	160	-13.755	25.649	33.182
	ATOM	526	HG2	MET	160	-14.292	24.405	32.009
	ATOM	527	SD	MET	160	-15.803	26.255	32.109
	ATOM	528	CE	MET	160	-15.256	27.848	32.785
	ATOM	529	HE1	MET	160	-16.105	28.530	32.842
55	ATOM	530	HE2	MET	160	-14.844	27.698	33.782
	ATOM	531	HE3	MET	160	-14.491	28.276	32.136
	ATOM	532	C	MET	160	-10.959	26.053	30.174
	ATOM	533	O	MET	160	-10.572	25.421	29.194
	ATOM	534	N	VAL	161	-10.678	27.353	30.356
60	ATOM	535	HN	VAL	161	-11.032	27.849	31.187
	ATOM	536	CA	VAL	161	-9.885	28.043	29.393
	ATOM	537	HA	VAL	161	-10.403	27.905	28.444
	ATOM	538	CB	VAL	161	-9.691	29.495	29.724
	ATOM	539	HB	VAL	161	-9.036	29.936	28.973
65	ATOM	540	CG1	VAL	161	-11.065	30.186	29.710
	ATOM	541	HG1	VAL	161	-10.944	31.243	29.948
	ATOM	542	HG1	VAL	161	-11.513	30.087	28.721
	ATOM	543	HG1	VAL	161	-11.715	29.720	30.451

	ATOM	544	CG2	VAL	161	-8.949	29.606	31.066
	ATOM	545	HG2	VAL	161	-8.803	30.657	31.316
	ATOM	546	HG2	VAL	161	-9.538	29.125	31.848
	ATOM	547	HG2	VAL	161	-7.980	29.113	30.988
	ATOM	548	C	VAL	161	-8.553	27.384	29.439
	ATOM	549	O	VAL	161	-7.872	27.249	28.423
	ATOM	550	N	GLY	162	-8.163	26.922	30.642
	ATOM	551	HN	GLY	162	-8.791	27.003	31.455
	ATOM	552	CA	GLY	162	-6.879	26.320	30.788
	ATOM	553	HA1	GLY	162	-6.820	25.592	29.979
	ATOM	554	HA2	GLY	162	-6.893	25.872	31.781
	ATOM	555	C	GLY	162	-5.917	27.443	30.653
	ATOM	556	O	GLY	162	-5.095	27.471	29.738
	ATOM	557	N	HIS	163	-5.986	28.417	31.580
	ATOM	558	HN	HIS	163	-6.644	28.363	32.371
	ATOM	559	CA	HIS	163	-5.105	29.529	31.417
	ATOM	560	HA	HIS	163	-4.633	29.544	30.434
	ATOM	561	ND1	HIS	163	-4.408	32.895	32.061
	ATOM	562	HD1	HIS	163	-4.423	32.809	33.088
	ATOM	563	CG	HIS	163	-5.031	32.063	31.157
	ATOM	564	NE2	HIS	163	-3.941	33.690	30.038
	ATOM	565	HE2	HIS	163	-3.566	34.274	29.276
	ATOM	566	CD2	HIS	163	-4.736	32.563	29.927
	ATOM	567	HD2	HIS	163	-5.079	32.135	28.985
	ATOM	568	CE1	HIS	163	-3.771	33.850	31.338
	ATOM	569	HE1	HIS	163	-3.186	34.657	31.779
	ATOM	570	CB	HIS	163	-5.851	30.870	31.539
	ATOM	571	HB1	HIS	163	-6.161	30.997	32.576
	ATOM	572	HB2	HIS	163	-6.720	30.840	30.881
	ATOM	573	C	HIS	163	-3.990	29.528	32.424
	ATOM	574	O	HIS	163	-3.946	30.412	33.279
	ATOM	575	N	PRO	164	-3.086	28.577	32.396
	ATOM	576	CA	PRO	164	-1.916	28.762	33.206
	ATOM	577	HA	PRO	164	-2.224	29.395	34.038
	ATOM	578	CD	PRO	164	-3.499	27.180	32.416
	ATOM	579	HD1	PRO	164	-3.821	26.952	31.400
	ATOM	580	HD2	PRO	164	-4.310	27.120	33.142
	ATOM	581	CB	PRO	164	-1.484	27.380	33.711
	ATOM	582	HB1	PRO	164	-1.775	27.364	34.761
	ATOM	583	HB2	PRO	164	-0.406	27.351	33.553
	ATOM	584	CG	PRO	164	-2.261	26.386	32.840
	ATOM	585	HG1	PRO	164	-2.527	25.494	33.408
	ATOM	586	HG2	PRO	164	-1.668	26.071	31.981
	ATOM	587	C	PRO	164	-0.906	29.419	32.324
	ATOM	588	O	PRO	164	-1.124	29.479	31.114
	ATOM	589	N	VAL	165	0.192	29.930	32.897
	ATOM	590	HN	VAL	165	0.289	29.907	33.923
	ATOM	591	CA	VAL	165	1.230	30.507	32.104
	ATOM	592	HA	VAL	165	0.798	30.606	31.109
	ATOM	593	CB	VAL	165	1.744	31.775	32.701
	ATOM	594	HB	VAL	165	2.116	31.563	33.703
	ATOM	595	CG1	VAL	165	2.876	32.311	31.816
	ATOM	596	HG1	VAL	165	3.261	33.239	32.240
	ATOM	597	HG1	VAL	165	3.678	31.575	31.765
	ATOM	598	HG1	VAL	165	2.494	32.502	30.813
	ATOM	599	CG2	VAL	165	0.563	32.741	32.876
	ATOM	600	HG2	VAL	165	0.919	33.675	33.312
	ATOM	601	HG2	VAL	165	0.111	32.943	31.905
	ATOM	602	HG2	VAL	165	-0.178	32.293	33.536
	ATOM	603	C	VAL	165	2.349	29.530	32.175
	ATOM	604	O	VAL	165	2.786	29.163	33.262
	ATOM	605	N	ILE	166	2.834	29.042	31.023
	ATOM	606	HN	ILE	166	2.452	29.317	30.107
	ATOM	607	CA	ILE	166	3.910	28.121	31.152
	ATOM	608	HA	ILE	166	4.101	27.964	32.213
	ATOM	609	CB	ILE	166	3.608	26.763	30.571
	ATOM	610	HB	ILE	166	2.794	26.288	31.118
	ATOM	611	CG2	ILE	166	3.192	26.890	29.088

	ATOM	612	HG2	ILE	166	2.977	25.901	28.685
	ATOM	613	HG2	ILE	166	2.301	27.514	29.012
	ATOM	614	HG2	ILE	166	4.003	27.346	28.520
	ATOM	615	CG1	ILE	166	4.774	25.800	30.845
5	ATOM	616	HG1	ILE	166	5.104	25.833	31.884
	ATOM	617	HG1	ILE	166	5.649	26.024	30.236
	ATOM	618	CD1	ILE	166	4.406	24.346	30.555
	ATOM	619	HD1	ILE	166	5.263	23.705	30.765
	ATOM	620	HD1	ILE	166	3.569	24.050	31.187
10	ATOM	621	HD1	ILE	166	4.124	24.244	29.507
	ATOM	622	C	ILE	166	5.102	28.703	30.488
	ATOM	623	O	ILE	166	5.193	28.742	29.262
	ATOM	624	N	PHE	167	6.061	29.220	31.275
	ATOM	625	HN	PHE	167	5.967	29.345	32.293
15	ATOM	626	CA	PHE	167	7.217	29.573	30.535
	ATOM	627	HA	PHE	167	6.831	29.904	29.571
	ATOM	628	CB	PHE	167	7.966	30.866	30.928
	ATOM	629	HB1	PHE	167	7.351	31.709	30.612
	ATOM	630	HB2	PHE	167	8.926	30.859	30.412
20	ATOM	631	CG	PHE	167	8.264	31.079	32.373
	ATOM	632	CD1	PHE	167	7.278	31.435	33.267
	ATOM	633	HD1	PHE	167	6.250	31.539	32.919
	ATOM	634	CD2	PHE	167	9.558	30.994	32.814
	ATOM	635	HD2	PHE	167	10.354	30.747	32.112
25	ATOM	636	CE1	PHE	167	7.569	31.660	34.590
	ATOM	637	HE1	PHE	167	6.776	31.926	35.289
	ATOM	638	CE2	PHE	167	9.859	31.219	34.134
	ATOM	639	HE2	PHE	167	10.890	31.135	34.478
	ATOM	640	CZ	PHE	167	8.865	31.550	35.026
30	ATOM	641	HZ	PHE	167	9.106	31.723	36.074
	ATOM	642	C	PHE	167	8.002	28.333	30.471
	ATOM	643	O	PHE	167	8.859	28.019	31.296
	ATOM	644	N	TYR	168	7.625	27.556	29.446
	ATOM	645	HN	TYR	168	6.935	27.914	28.769
35	ATOM	646	CA	TYR	168	8.154	26.252	29.272
	ATOM	647	HA	TYR	168	7.814	25.630	30.099
	ATOM	648	CB	TYR	168	8.061	25.640	27.863
	ATOM	649	HB1	TYR	168	8.769	24.812	27.823
	ATOM	650	HB2	TYR	168	8.321	26.423	27.151
40	ATOM	651	CG	TYR	168	6.765	25.096	27.423
	ATOM	652	CD1	TYR	168	6.214	24.010	28.059
	ATOM	653	HD1	TYR	168	6.734	23.563	28.907
	ATOM	654	CD2	TYR	168	6.164	25.598	26.300
	ATOM	655	HD2	TYR	168	6.631	26.412	25.744
45	ATOM	656	CE1	TYR	168	5.018	23.478	27.644
	ATOM	657	HE1	TYR	168	4.569	22.639	28.177
	ATOM	658	CE2	TYR	168	4.974	25.071	25.879
	ATOM	659	HE2	TYR	168	4.479	25.489	25.003
	ATOM	660	CZ	TYR	168	4.397	24.021	26.547
50	ATOM	661	OH	TYR	168	3.166	23.496	26.097
	ATOM	662	HH	TYR	168	2.446	24.232	26.131
	ATOM	663	C	TYR	168	9.607	26.344	29.265
	ATOM	664	O	TYR	168	10.301	25.843	30.143
	ATOM	665	N	ILE	169	10.119	27.032	28.248
55	ATOM	666	HN	ILE	169	9.605	27.716	27.673
	ATOM	667	CA	ILE	169	11.469	26.681	28.081
	ATOM	668	HA	ILE	169	11.592	25.644	28.393
	ATOM	669	CB	ILE	169	11.935	26.582	26.652
	ATOM	670	HB	ILE	169	11.252	25.950	26.085
60	ATOM	671	CG2	ILE	169	11.969	27.977	26.023
	ATOM	672	HG2	ILE	169	12.307	27.902	24.989
	ATOM	673	HG2	ILE	169	10.970	28.412	26.047
	ATOM	674	HG2	ILE	169	12.655	28.612	26.583
	ATOM	675	CG1	ILE	169	13.295	25.868	26.602
65	ATOM	676	HG1	ILE	169	13.327	24.957	27.200
	ATOM	677	HG1	ILE	169	14.119	26.481	26.968
	ATOM	678	CD1	ILE	169	13.704	25.441	25.194
	ATOM	679	HD1	ILE	169	14.673	24.944	25.231

```
ATOM    680  HD1 ILE   169      12.958  24.755  24.791
ATOM    681  HD1 ILE   169      13.772  26.320  24.553
ATOM    682  C   ILE   169      12.414  27.491  28.858
ATOM    683  O   ILE   169      12.688  28.655  28.578
ATOM    684  N   MET   170      12.900  26.847  29.920
ATOM    685  HN  MET   170      12.428  26.010  30.289
ATOM    686  CA  MET   170      14.075  27.338  30.526
ATOM    687  HA  MET   170      14.282  28.370  30.240
ATOM    688  CB  MET   170      14.089  27.212  32.049
ATOM    689  HB1 MET   170      13.937  26.178  32.361
ATOM    690  HB2 MET   170      13.302  27.813  32.503
ATOM    691  CG  MET   170      15.421  27.679  32.631
ATOM    692  HG1 MET   170      16.291  27.235  32.147
ATOM    693  HG2 MET   170      15.541  27.448  33.690
ATOM    694  SD  MET   170      15.682  29.472  32.510
ATOM    695  CE  MET   170      16.169  29.427  30.762
ATOM    696  HE1 MET   170      16.394  30.438  30.421
ATOM    697  HE2 MET   170      17.054  28.800  30.646
ATOM    698  HE3 MET   170      15.353  29.016  30.167
ATOM    699  C   MET   170      15.057  26.366  29.975
ATOM    700  O   MET   170      15.375  25.353  30.598
ATOM    701  N   VAL   171      15.540  26.639  28.752
ATOM    702  HN  VAL   171      15.301  27.518  28.272
ATOM    703  CA  VAL   171      16.395  25.677  28.138
ATOM    704  HA  VAL   171      16.078  24.685  28.460
ATOM    705  CB  VAL   171      16.369  25.696  26.637
ATOM    706  HB  VAL   171      15.335  25.611  26.304
ATOM    707  CG1 VAL   171      16.975  27.021  26.149
ATOM    708  HG1 VAL   171      16.961  27.048  25.060
ATOM    709  HG1 VAL   171      16.390  27.854  26.540
ATOM    710  HG1 VAL   171      18.003  27.103  26.502
ATOM    711  CG2 VAL   171      17.107  24.448  26.125
ATOM    712  HG2 VAL   171      17.099  24.442  25.035
ATOM    713  HG2 VAL   171      18.137  24.463  26.481
ATOM    714  HG2 VAL   171      16.608  23.553  26.496
ATOM    715  C   VAL   171      17.791  25.952  28.574
ATOM    716  O   VAL   171      18.213  27.101  28.701
ATOM    717  N   ASP   172      18.537  24.868  28.839
ATOM    718  HN  ASP   172      18.126  23.932  28.714
ATOM    719  CA  ASP   172      19.886  24.984  29.288
ATOM    720  HA  ASP   172      19.974  25.936  29.810
ATOM    721  CB  ASP   172      20.295  23.806  30.189
ATOM    722  HB1 ASP   172      20.368  22.910  29.573
ATOM    723  HB2 ASP   172      19.534  23.679  30.958
ATOM    724  CG  ASP   172      21.638  24.127  30.819
ATOM    725  OD1 ASP   172      21.805  25.272  31.320
ATOM    726  OD2 ASP   172      22.512  23.221  30.823
ATOM    727  C   ASP   172      20.766  24.938  28.077
ATOM    728  O   ASP   172      21.788  24.254  28.079
ATOM    729  N   ASP   173      20.413  25.705  27.026
ATOM    730  HN  ASP   173      19.576  26.302  27.096
ATOM    731  CA  ASP   173      21.177  25.711  25.809
ATOM    732  HA  ASP   173      20.653  26.309  25.065
ATOM    733  CB  ASP   173      22.582  26.326  25.965
ATOM    734  HB1 ASP   173      23.195  25.647  26.557
ATOM    735  HB2 ASP   173      22.485  27.288  26.470
ATOM    736  CG  ASP   173      23.186  26.514  24.577
ATOM    737  OD1 ASP   173      23.330  25.502  23.840
ATOM    738  OD2 ASP   173      23.521  27.679  24.237
ATOM    739  C   ASP   173      21.325  24.304  25.323
ATOM    740  O   ASP   173      22.406  23.721  25.390
ATOM    741  N   VAL   174      20.215  23.721  24.827
ATOM    742  HN  VAL   174      19.338  24.259  24.797
ATOM    743  CA  VAL   174      20.223  22.371  24.339
ATOM    744  HA  VAL   174      20.895  21.773  24.955
ATOM    745  CB  VAL   174      18.875  21.712  24.363
ATOM    746  HB  VAL   174      18.968  20.718  23.927
ATOM    747  CG1 VAL   174      18.404  21.616  25.824
```

	ATOM	748	HG1	VAL	174	17.425	21.139	25.861
	ATOM	749	HG1	VAL	174	19.117	21.024	26.398
	ATOM	750	HG1	VAL	174	18.336	22.617	26.251
	ATOM	751	CG2	VAL	174	17.923	22.499	23.446
5	ATOM	752	HG2	VAL	174	16.939	22.031	23.454
	ATOM	753	HG2	VAL	174	17.839	23.526	23.803
	ATOM	754	HG2	VAL	174	18.316	22.500	22.429
	ATOM	755	C	VAL	174	20.696	22.366	22.921
	ATOM	756	O	VAL	174	20.953	23.413	22.328
10	ATOM	757	N	SER	175	20.822	21.156	22.341
	ATOM	758	HN	SER	175	20.560	20.313	22.873
	ATOM	759	CA	SER	175	21.314	21.015	21.004
	ATOM	760	HA	SER	175	22.165	21.680	20.855
	ATOM	761	CB	SER	175	21.834	19.604	20.671
15	ATOM	762	HB1	SER	175	22.615	19.309	21.371
	ATOM	763	HB2	SER	175	22.248	19.577	19.663
	ATOM	764	OG	SER	175	20.783	18.655	20.748
	ATOM	765	HG	SER	175	19.906	19.132	21.002
	ATOM	766	C	SER	175	20.236	21.368	20.034
20	ATOM	767	O	SER	175	19.112	21.700	20.408
	ATOM	768	N	ARG	176	20.596	21.302	18.740
	ATOM	769	HN	ARG	176	21.539	20.946	18.530
	ATOM	770	CA	ARG	176	19.777	21.686	17.628
	ATOM	771	HA	ARG	176	19.491	22.736	17.692
25	ATOM	772	CB	ARG	176	20.519	21.457	16.302
	ATOM	773	HB1	ARG	176	21.432	22.049	16.237
	ATOM	774	HB2	ARG	176	19.908	21.725	15.440
	ATOM	775	CG	ARG	176	20.926	19.992	16.118
	ATOM	776	HG1	ARG	176	20.053	19.434	15.781
30	ATOM	777	HG2	ARG	176	21.278	19.611	17.076
	ATOM	778	CD	ARG	176	22.041	19.774	15.093
	ATOM	779	HD1	ARG	176	22.352	18.731	15.148
	ATOM	780	HD2	ARG	176	22.867	20.438	15.345
	ATOM	781	NE	ARG	176	21.499	20.094	13.745
35	ATOM	782	HE	ARG	176	20.490	20.256	13.615
	ATOM	783	CZ	ARG	176	22.351	20.171	12.682
	ATOM	784	NH1	ARG	176	23.689	19.966	12.865
	ATOM	785	HH1	ARG	176	24.333	20.023	12.064
	ATOM	786	HH1	ARG	176	24.053	19.753	13.805
40	ATOM	787	NH2	ARG	176	21.872	20.454	11.437
	ATOM	788	HH2	ARG	176	22.518	20.512	10.637
	ATOM	789	HH2	ARG	176	20.863	20.611	11.297
	ATOM	790	C	ARG	176	18.520	20.876	17.575
	ATOM	791	O	ARG	176	17.433	21.426	17.406
45	ATOM	792	N	MET	177	18.617	19.544	17.731
	ATOM	793	HN	MET	177	19.518	19.105	17.967
	ATOM	794	CA	MET	177	17.434	18.752	17.561
	ATOM	795	HA	MET	177	16.992	18.939	16.583
	ATOM	796	CB	MET	177	17.688	17.234	17.581
50	ATOM	797	HB1	MET	177	17.922	16.864	18.579
	ATOM	798	HB2	MET	177	18.522	16.943	16.942
	ATOM	799	CG	MET	177	16.475	16.432	17.097
	ATOM	800	HG1	MET	177	16.079	16.922	16.208
	ATOM	801	HG2	MET	177	15.736	16.422	17.898
55	ATOM	802	SD	MET	177	16.817	14.701	16.654
	ATOM	803	CE	MET	177	17.175	14.161	18.350
	ATOM	804	HE1	MET	177	17.422	13.099	18.349
	ATOM	805	HE2	MET	177	18.019	14.730	18.741
	ATOM	806	HE3	MET	177	16.301	14.330	18.978
60	ATOM	807	C	MET	177	16.426	19.091	18.615
	ATOM	808	O	MET	177	15.230	19.136	18.332
	ATOM	809	N	PRO	178	16.833	19.309	19.830
	ATOM	810	CA	PRO	178	15.853	19.648	20.824
	ATOM	811	HA	PRO	178	15.036	18.927	20.853
65	ATOM	812	CD	PRO	178	17.943	18.564	20.396
	ATOM	813	HD1	PRO	178	18.829	19.169	20.205
	ATOM	814	HD2	PRO	178	17.955	17.611	19.868
	ATOM	815	CB	PRO	178	16.566	19.506	22.168

ATOM	816	HB1	PRO	178	15.870	19.206	22.951
ATOM	817	HB2	PRO	178	17.023	20.448	22.470
ATOM	818	CG	PRO	178	17.623	18.420	21.894
ATOM	819	HG1	PRO	178	17.126	17.485	22.152
ATOM	820	HG2	PRO	178	18.454	18.676	22.551
ATOM	821	C	PRO	178	15.239	20.991	20.570
ATOM	822	O	PRO	178	14.067	21.189	20.890
ATOM	823	N	LEU	179	16.014	21.921	19.989
ATOM	824	HN	LEU	179	16.980	21.679	19.727
ATOM	825	CA	LEU	179	15.528	23.241	19.724
ATOM	826	HA	LEU	179	15.187	23.666	20.668
ATOM	827	CB	LEU	179	16.584	24.129	19.044
ATOM	828	HB1	LEU	179	16.153	25.119	18.897
ATOM	829	HB2	LEU	179	16.845	23.676	18.087
ATOM	830	CG	LEU	179	17.890	24.305	19.845
ATOM	831	HG	LEU	179	18.373	23.344	20.019
ATOM	832	CD2	LEU	179	17.630	24.786	21.280
ATOM	833	HD2	LEU	179	18.579	24.896	21.804
ATOM	834	HD2	LEU	179	17.116	25.748	21.253
ATOM	835	HD2	LEU	179	17.009	24.058	21.801
ATOM	836	CD1	LEU	179	18.881	25.203	19.088
ATOM	837	HD1	LEU	179	19.794	25.312	19.674
ATOM	838	HD1	LEU	179	19.119	24.752	18.125
ATOM	839	HD1	LEU	179	18.434	26.184	18.928
ATOM	840	C	LEU	179	14.403	23.127	18.747
ATOM	841	O	LEU	179	13.360	23.759	18.912
ATOM	842	N	ILE	180	14.597	22.304	17.698
ATOM	843	HN	ILE	180	15.468	21.757	17.638
ATOM	844	CA	ILE	180	13.609	22.175	16.662
ATOM	845	HA	ILE	180	13.363	23.164	16.275
ATOM	846	CB	ILE	180	14.045	21.341	15.484
ATOM	847	HB	ILE	180	13.225	21.314	14.767
ATOM	848	CG2	ILE	180	15.289	22.001	14.868
ATOM	849	HG2	ILE	180	15.625	21.415	14.012
ATOM	850	HG2	ILE	180	15.041	23.011	14.542
ATOM	851	HG2	ILE	180	16.084	22.045	15.612
ATOM	852	CG1	ILE	180	14.265	19.876	15.882
ATOM	853	HG1	ILE	180	13.449	19.458	16.470
ATOM	854	HG1	ILE	180	15.160	19.718	16.484
ATOM	855	CD1	ILE	180	14.418	18.937	14.688
ATOM	856	HD1	ILE	180	14.570	17.918	15.043
ATOM	857	HD1	ILE	180	13.517	18.977	14.076
ATOM	858	HD1	ILE	180	15.276	19.245	14.090
ATOM	859	C	ILE	180	12.382	21.538	17.227
ATOM	860	O	ILE	180	11.264	21.896	16.861
ATOM	861	N	GLU	181	12.562	20.579	18.155
ATOM	862	HN	GLU	181	13.513	20.357	18.483
ATOM	863	CA	GLU	181	11.440	19.864	18.692
ATOM	864	HA	GLU	181	10.954	19.323	17.880
ATOM	865	CB	GLU	181	11.850	18.883	19.805
ATOM	866	HB1	GLU	181	10.946	18.441	20.225
ATOM	867	HB2	GLU	181	12.395	19.437	20.569
ATOM	868	CG	GLU	181	12.749	17.741	19.325
ATOM	869	HG1	GLU	181	13.188	17.272	20.205
ATOM	870	HG2	GLU	181	13.518	18.172	18.684
ATOM	871	CD	GLU	181	11.880	16.760	18.556
ATOM	872	OE1	GLU	181	11.057	16.057	19.201
ATOM	873	OE2	GLU	181	12.028	16.705	17.307
ATOM	875	C	GLU	181	10.498	20.849	19.301
ATOM	876	O	GLU	181	9.297	20.797	19.038
ATOM	877	N	LEU	182	11.011	21.789	20.123
ATOM	878	HN	LEU	182	12.019	21.823	20.331
ATOM	879	CA	LEU	182	10.104	22.736	20.697
ATOM	880	HA	LEU	182	9.331	22.163	21.209
ATOM	881	CB	LEU	182	10.717	23.682	21.744
ATOM	882	HB1	LEU	182	10.048	24.499	22.015
ATOM	883	HB2	LEU	182	11.640	24.149	21.399
ATOM	884	CG	LEU	182	11.067	22.965	23.056

ATOM	885	HG	LEU	182	10.229	22.368	23.415
ATOM	886	CD2	LEU	182	11.230	23.973	24.202
ATOM	887	HD2	LEU	182	11.478	23.442	25.121
ATOM	888	HD2	LEU	182	12.031	24.673	23.960
ATOM	889	HD2	LEU	182	10.299	24.522	24.339
ATOM	890	CD1	LEU	182	12.267	22.021	22.871
ATOM	891	HD1	LEU	182	12.491	21.528	23.817
ATOM	892	HD1	LEU	182	12.027	21.270	22.118
ATOM	893	HD1	LEU	182	13.135	22.595	22.547
ATOM	894	C	LEU	182	9.546	23.540	19.568
ATOM	895	O	LEU	182	8.354	23.829	19.549
ATOM	896	N	GLY	183	10.423	23.888	18.602
ATOM	897	HN	GLY	183	11.397	23.595	18.764
ATOM	898	CA	GLY	183	10.193	24.611	17.376
ATOM	899	HA1	GLY	183	10.272	23.909	16.546
ATOM	900	HA2	GLY	183	10.949	25.392	17.293
ATOM	901	C	GLY	183	8.852	25.269	17.284
ATOM	902	O	GLY	183	8.682	26.430	17.658
ATOM	903	N	PRO	184	7.892	24.554	16.761
ATOM	904	CA	PRO	184	6.596	25.124	16.533
ATOM	905	HA	PRO	184	6.630	25.933	15.804
ATOM	906	CD	PRO	184	8.149	23.402	15.913
ATOM	907	HD1	PRO	184	8.339	22.579	16.602
ATOM	908	HD2	PRO	184	9.018	23.677	15.315
ATOM	909	CB	PRO	184	5.789	24.027	15.842
ATOM	910	HB1	PRO	184	5.048	24.453	15.166
ATOM	911	HB2	PRO	184	5.261	23.411	16.571
ATOM	912	CG	PRO	184	6.865	23.220	15.080
ATOM	913	HG1	PRO	184	6.910	23.684	14.095
ATOM	914	HG2	PRO	184	6.487	22.198	15.070
ATOM	915	C	PRO	184	6.011	25.688	17.781
ATOM	916	O	PRO	184	5.454	26.784	17.734
ATOM	917	N	LEU	185	6.103	24.949	18.894
ATOM	918	HN	LEU	185	6.491	23.996	18.840
ATOM	919	CA	LEU	185	5.673	25.458	20.151
ATOM	920	HA	LEU	185	4.675	25.876	20.020
ATOM	921	CB	LEU	185	5.599	24.371	21.228
ATOM	922	HB1	LEU	185	5.361	24.768	22.214
ATOM	923	HB2	LEU	185	6.536	23.826	21.344
ATOM	924	CG	LEU	185	4.525	23.305	20.930
ATOM	925	HG	LEU	185	4.538	22.508	21.673
ATOM	926	CD2	LEU	185	4.850	22.515	19.651
ATOM	927	HD2	LEU	185	4.071	21.773	19.474
ATOM	928	HD2	LEU	185	4.899	23.199	18.804
ATOM	929	HD2	LEU	185	5.809	22.012	19.768
ATOM	930	CD1	LEU	185	3.111	23.915	20.934
ATOM	931	HD1	LEU	185	2.378	23.137	20.721
ATOM	932	HD1	LEU	185	2.905	24.350	21.912
ATOM	933	HD1	LEU	185	3.048	24.691	20.171
ATOM	934	C	LEU	185	6.646	26.513	20.577
ATOM	935	O	LEU	185	6.236	27.546	21.103
ATOM	936	N	ARG	186	7.964	26.292	20.360
ATOM	937	HN	ARG	186	8.286	25.438	19.883
ATOM	938	CA	ARG	186	8.900	27.280	20.814
ATOM	939	HA	ARG	186	8.472	27.795	21.674
ATOM	940	CB	ARG	186	10.277	26.738	21.260
ATOM	941	HB1	ARG	186	10.104	25.959	22.003
ATOM	942	HB2	ARG	186	10.840	27.568	21.688
ATOM	943	CG	ARG	186	11.149	26.124	20.163
ATOM	944	HG1	ARG	186	11.235	26.770	19.289
ATOM	945	HG2	ARG	186	10.757	25.172	19.803
ATOM	946	CD	ARG	186	12.579	25.849	20.638
ATOM	947	HD1	ARG	186	13.127	25.518	19.756
ATOM	948	HD2	ARG	186	12.495	25.074	21.399
ATOM	949	NE	ARG	186	13.083	27.142	21.181
ATOM	950	HE	ARG	186	12.411	27.863	21.481
ATOM	951	CZ	ARG	186	14.421	27.384	21.287
ATOM	952	NH1	ARG	186	15.325	26.443	20.885

ATOM	953	HH1	ARG	186	16.334	26.630	20.967
ATOM	954	HH1	ARG	186	14.997	25.545	20.500
ATOM	955	NH2	ARG	186	14.857	28.579	21.778
ATOM	956	HH2	ARG	186	15.866	28.765	21.859
ATOM	957	HH2	ARG	186	14.176	29.296	22.068
ATOM	958	C	ARG	186	9.149	28.244	19.703
ATOM	959	O	ARG	186	10.285	28.605	19.399
ATOM	960	N	SER	187	8.069	28.677	19.042
ATOM	961	HN	SER	187	7.141	28.274	19.235
ATOM	962	CA	SER	187	8.223	29.702	18.069
ATOM	963	HA	SER	187	8.998	30.409	18.365
ATOM	964	CB	SER	187	8.560	29.160	16.673
ATOM	965	HB1	SER	187	7.735	28.544	16.313
ATOM	966	HB2	SER	187	9.466	28.557	16.725
ATOM	967	OG	SER	187	8.764	30.244	15.780
ATOM	968	HG	SER	187	9.409	30.924	16.207
ATOM	969	C	SER	187	6.886	30.335	18.027
ATOM	970	O	SER	187	6.533	30.969	17.033
ATOM	971	N	PHE	188	6.153	30.173	19.155
ATOM	972	HN	PHE	188	6.595	29.660	19.931
ATOM	973	CA	PHE	188	4.814	30.651	19.366
ATOM	974	HA	PHE	188	4.707	31.113	20.347
ATOM	975	CB	PHE	188	4.272	31.696	18.348
ATOM	976	HB1	PHE	188	3.199	31.542	18.239
ATOM	977	HB2	PHE	188	4.781	31.541	17.397
ATOM	978	CG	PHE	188	4.485	33.115	18.746
ATOM	979	CD1	PHE	188	5.654	33.800	18.496
ATOM	980	HD1	PHE	188	6.477	33.300	17.987
ATOM	981	CD2	PHE	188	3.454	33.771	19.376
ATOM	982	HD2	PHE	188	2.521	33.241	19.569
ATOM	983	CE1	PHE	188	5.786	35.113	18.885
ATOM	984	HE1	PHE	188	6.716	35.646	18.689
ATOM	985	CE2	PHE	188	3.578	35.081	19.768
ATOM	986	HE2	PHE	188	2.751	35.583	20.270
ATOM	987	CZ	PHE	188	4.750	35.755	19.521
ATOM	988	HZ	PHE	188	4.858	36.795	19.829
ATOM	989	C	PHE	188	3.825	29.546	19.282
ATOM	990	O	PHE	188	3.879	28.548	20.002
ATOM	991	N	LYS	189	2.890	29.761	18.338
ATOM	992	HN	LYS	189	3.029	30.589	17.742
ATOM	993	CA	LYS	189	1.726	28.977	18.066
ATOM	994	HA	LYS	189	1.014	29.568	17.491
ATOM	995	CB	LYS	189	1.923	27.777	17.123
ATOM	996	HB1	LYS	189	2.382	26.942	17.652
ATOM	997	HB2	LYS	189	2.568	28.047	16.287
ATOM	998	CG	LYS	189	0.578	27.306	16.558
ATOM	999	HG1	LYS	189	-0.134	27.007	17.327
ATOM	1000	HG2	LYS	189	0.663	26.444	15.896
ATOM	1001	CD	LYS	189	-0.149	28.380	15.731
ATOM	1002	HD1	LYS	189	-0.976	27.901	15.207
ATOM	1003	HD2	LYS	189	0.564	28.802	15.023
ATOM	1004	CE	LYS	189	-0.733	29.545	16.543
ATOM	1005	HE1	LYS	189	0.051	30.062	17.095
ATOM	1006	HE2	LYS	189	-1.472	29.184	17.258
ATOM	1007	NZ	LYS	189	-1.392	30.523	15.653
ATOM	1008	HZ1	LYS	189	-1.776	31.295	16.215
ATOM	1009	HZ2	LYS	189	-0.704	30.896	14.983
ATOM	1010	HZ3	LYS	189	-2.155	30.060	15.138
ATOM	1011	C	LYS	189	1.098	28.557	19.348
ATOM	1012	O	LYS	189	0.681	27.411	19.516
ATOM	1013	N	VAL	190	1.082	29.508	20.299
ATOM	1014	HN	VAL	190	1.621	30.366	20.115
ATOM	1015	CA	VAL	190	0.383	29.431	21.544
ATOM	1016	HA	VAL	190	-0.655	29.650	21.294
ATOM	1017	CB	VAL	190	0.344	28.073	22.204
ATOM	1018	HB	VAL	190	0.112	27.289	21.483
ATOM	1019	CG1	VAL	190	1.696	27.728	22.847
ATOM	1020	HG1	VAL	190	1.637	26.745	23.314

	ATOM	1021	HG1	VAL	190	2.472	27.720	22.081
	ATOM	1022	HG1	VAL	190	1.940	28.475	23.603
	ATOM	1023	CG2	VAL	190	-0.856	28.072	23.164
	ATOM	1024	HG2	VAL	190	-0.922	27.106	23.664
5	ATOM	1025	HG2	VAL	190	-0.728	28.858	23.908
	ATOM	1026	HG2	VAL	190	-1.772	28.252	22.601
	ATOM	1027	C	VAL	190	1.024	30.470	22.409
	ATOM	1028	O	VAL	190	2.221	30.413	22.683
	ATOM	1029	N	PHE	191	0.225	31.465	22.847
10	ATOM	1030	HN	PHE	191	-0.778	31.392	22.631
	ATOM	1031	CA	PHE	191	0.656	32.620	23.591
	ATOM	1032	HA	PHE	191	1.482	33.101	23.067
	ATOM	1033	CB	PHE	191	-0.475	33.640	23.756
	ATOM	1034	HB1	PHE	191	-0.053	34.492	24.289
15	ATOM	1035	HB2	PHE	191	-1.260	33.146	24.328
	ATOM	1036	CG	PHE	191	-0.925	34.005	22.383
	ATOM	1037	CD1	PHE	191	-0.158	34.830	21.595
	ATOM	1038	HD1	PHE	191	0.788	35.216	21.972
	ATOM	1039	CD2	PHE	191	-2.123	33.528	21.902
20	ATOM	1040	HD2	PHE	191	-2.735	32.876	22.527
	ATOM	1041	CE1	PHE	191	-0.581	35.171	20.334
	ATOM	1042	HE1	PHE	191	0.028	35.825	19.711
	ATOM	1043	CE2	PHE	191	-2.556	33.865	20.643
	ATOM	1044	HE2	PHE	191	-3.506	33.486	20.268
25	ATOM	1045	CZ	PHE	191	-1.778	34.684	19.860
	ATOM	1046	HZ	PHE	191	-2.111	34.950	18.856
	ATOM	1047	C	PHE	191	1.107	32.195	24.950
	ATOM	1048	O	PHE	191	1.908	32.867	25.601
	ATOM	1049	N	LYS	192	0.571	31.046	25.387
30	ATOM	1050	HN	LYS	192	-0.023	30.539	24.716
	ATOM	1051	CA	LYS	192	0.730	30.441	26.676
	ATOM	1052	HA	LYS	192	0.271	31.074	27.436
	ATOM	1053	CB	LYS	192	0.157	29.021	26.625
	ATOM	1054	HB1	LYS	192	0.873	28.398	26.088
35	ATOM	1055	HB2	LYS	192	-0.796	29.071	26.100
	ATOM	1056	CG	LYS	192	-0.114	28.323	27.951
	ATOM	1057	HG1	LYS	192	-0.762	28.925	28.589
	ATOM	1058	HG2	LYS	192	0.809	28.141	28.499
	ATOM	1059	CD	LYS	192	-0.800	26.971	27.738
40	ATOM	1060	HD1	LYS	192	-1.146	26.607	28.705
	ATOM	1061	HD2	LYS	192	-0.073	26.284	27.305
	ATOM	1062	CE	LYS	192	-2.012	27.014	26.799
	ATOM	1063	HE1	LYS	192	-2.144	26.052	26.305
	ATOM	1064	HE2	LYS	192	-1.874	27.780	26.036
45	ATOM	1065	NZ	LYS	192	-3.244	27.325	27.562
	ATOM	1066	HZ1	LYS	192	-4.048	27.351	26.919
	ATOM	1067	HZ2	LYS	192	-3.398	26.600	28.276
	ATOM	1068	HZ3	LYS	192	-3.142	28.242	28.020
	ATOM	1069	C	LYS	192	2.187	30.279	26.980
50	ATOM	1070	O	LYS	192	2.606	30.457	28.122
	ATOM	1071	N	ILE	193	2.996	29.952	25.954
	ATOM	1072	HN	ILE	193	2.603	29.946	25.002
	ATOM	1073	CA	ILE	193	4.381	29.611	26.127
	ATOM	1074	HA	ILE	193	4.546	29.002	27.016
55	ATOM	1075	CB	ILE	193	4.902	28.846	24.948
	ATOM	1076	HB	ILE	193	4.735	29.444	24.052
	ATOM	1077	CG2	ILE	193	6.402	28.596	25.161
	ATOM	1078	HG2	ILE	193	6.802	28.040	24.313
	ATOM	1079	HG2	ILE	193	6.921	29.550	25.246
60	ATOM	1080	HG2	ILE	193	6.549	28.020	26.075
	ATOM	1081	CG1	ILE	193	4.067	27.578	24.687
	ATOM	1082	HG1	ILE	193	3.001	27.784	24.590
	ATOM	1083	HG1	ILE	193	4.155	26.840	25.485
	ATOM	1084	CD1	ILE	193	4.471	26.850	23.397
65	ATOM	1085	HD1	ILE	193	3.847	25.965	23.268
	ATOM	1086	HD1	ILE	193	4.336	27.516	22.546
	ATOM	1087	HD1	ILE	193	5.517	26.550	23.461
	ATOM	1088	C	ILE	193	5.253	30.833	26.271

ATOM	1089	O	ILE	193	5.089	31.833	25.576
ATOM	1090	N	LYS	194	6.213	30.772	27.222
ATOM	1091	HN	LYS	194	6.246	29.938	27.826
ATOM	1092	CA	LYS	194	7.192	31.807	27.438
ATOM	1093	HA	LYS	194	7.104	32.498	26.599
ATOM	1094	CB	LYS	194	7.012	32.605	28.750
ATOM	1095	HB1	LYS	194	7.934	33.154	28.946
ATOM	1096	HB2	LYS	194	6.807	31.899	29.555
ATOM	1097	CG	LYS	194	5.863	33.621	28.716
ATOM	1098	HG1	LYS	194	4.970	33.236	28.225
ATOM	1099	HG2	LYS	194	6.121	34.537	28.186
ATOM	1100	CD	LYS	194	5.412	34.062	30.117
ATOM	1101	HD1	LYS	194	4.663	33.398	30.550
ATOM	1102	HD2	LYS	194	4.967	35.057	30.126
ATOM	1103	CE	LYS	194	6.570	34.110	31.134
ATOM	1104	HE1	LYS	194	7.248	33.267	31.000
ATOM	1105	HE2	LYS	194	6.199	34.075	32.158
ATOM	1106	NZ	LYS	194	7.369	35.361	30.985
ATOM	1107	HZ1	LYS	194	8.134	35.365	31.676
ATOM	1108	HZ2	LYS	194	7.765	35.406	30.035
ATOM	1109	HZ3	LYS	194	6.761	36.178	31.142
ATOM	1110	C	LYS	194	8.530	31.130	27.477
ATOM	1111	O	LYS	194	8.866	30.363	28.379
ATOM	1112	N	PRO	195	9.272	31.379	26.438
ATOM	1113	CA	PRO	195	10.582	30.791	26.334
ATOM	1114	HA	PRO	195	10.568	29.829	26.847
ATOM	1115	CD	PRO	195	8.635	31.518	25.136
ATOM	1116	HD1	PRO	195	8.172	32.504	25.155
ATOM	1117	HD2	PRO	195	7.918	30.699	25.086
ATOM	1118	CB	PRO	195	10.801	30.506	24.844
ATOM	1119	HB1	PRO	195	10.608	29.439	24.733
ATOM	1120	HB2	PRO	195	11.837	30.786	24.656
ATOM	1121	CG	PRO	195	9.781	31.395	24.121
ATOM	1122	HG1	PRO	195	9.449	30.934	23.191
ATOM	1123	HG2	PRO	195	10.212	32.366	23.878
ATOM	1124	C	PRO	195	11.681	31.617	26.943
ATOM	1125	O	PRO	195	11.522	32.829	27.091
ATOM	1126	N	GLU	196	12.794	30.945	27.318
ATOM	1127	HN	GLU	196	12.765	29.917	27.259
ATOM	1128	CA	GLU	196	14.011	31.542	27.791
ATOM	1129	HA	GLU	196	14.120	32.488	27.261
ATOM	1130	CB	GLU	196	14.103	31.795	29.305
ATOM	1131	HB1	GLU	196	13.964	30.870	29.865
ATOM	1132	HB2	GLU	196	13.340	32.501	29.631
ATOM	1133	CG	GLU	196	15.470	32.372	29.683
ATOM	1134	HG1	GLU	196	15.666	33.261	29.085
ATOM	1135	HG2	GLU	196	16.243	31.627	29.494
ATOM	1136	CD	GLU	196	15.471	32.742	31.160
ATOM	1137	OE1	GLU	196	14.584	33.541	31.568
ATOM	1138	OE2	GLU	196	16.361	32.229	31.895
ATOM	1140	C	GLU	196	15.111	30.581	27.467
ATOM	1141	O	GLU	196	14.905	29.368	27.468
ATOM	1142	N	LYS	197	16.315	31.112	27.172
ATOM	1143	HN	LYS	197	16.431	32.135	27.194
ATOM	1144	CA	LYS	197	17.441	30.288	26.830
ATOM	1145	HA	LYS	197	17.260	29.285	27.217
ATOM	1146	CB	LYS	197	17.702	30.274	25.314
ATOM	1147	HB1	LYS	197	17.780	31.307	24.976
ATOM	1148	HB2	LYS	197	16.865	29.769	24.833
ATOM	1149	CG	LYS	197	18.980	29.555	24.868
ATOM	1150	HG1	LYS	197	18.992	28.509	25.174
ATOM	1151	HG2	LYS	197	19.877	30.013	25.285
ATOM	1152	CD	LYS	197	19.150	29.568	23.345
ATOM	1153	HD1	LYS	197	18.935	30.575	22.988
ATOM	1154	HD2	LYS	197	18.448	28.849	22.920
ATOM	1155	CE	LYS	197	20.548	29.193	22.846
ATOM	1156	HE1	LYS	197	21.268	29.266	23.660
ATOM	1157	HE2	LYS	197	20.853	29.867	22.045

	ATOM	1158	NZ	LYS	197	20.549	27.804	22.329
	ATOM	1159	HZ1	LYS	197	21.493	27.563	21.996
	ATOM	1160	HZ2	LYS	197	20.275	27.157	23.082
	ATOM	1161	HZ3	LYS	197	19.880	27.727	21.549
5	ATOM	1162	C	LYS	197	18.666	30.883	27.456
	ATOM	1163	O	LYS	197	18.825	32.101	27.507
	ATOM	1164	N	ARG	198	19.574	30.030	27.968
	ATOM	1165	HN	ARG	198	19.385	29.018	27.996
	ATOM	1166	CA	ARG	198	20.809	30.554	28.475
10	ATOM	1167	HA	ARG	198	20.676	31.636	28.498
	ATOM	1168	CB	ARG	198	21.118	30.083	29.903
	ATOM	1169	HB1	ARG	198	22.135	30.362	30.179
	ATOM	1170	HB2	ARG	198	21.021	28.999	29.970
	ATOM	1171	CG	ARG	198	20.142	30.727	30.894
15	ATOM	1172	HG1	ARG	198	19.146	30.700	30.453
	ATOM	1173	HG2	ARG	198	20.463	31.755	31.064
	ATOM	1174	CD	ARG	198	20.054	30.048	32.259
	ATOM	1175	HD1	ARG	198	20.265	28.986	32.130
	ATOM	1176	HD2	ARG	198	19.046	30.191	32.651
20	ATOM	1177	NE	ARG	198	21.057	30.673	33.162
	ATOM	1178	HE	ARG	198	21.903	31.115	32.776
	ATOM	1179	CZ	ARG	198	20.840	30.651	34.509
	ATOM	1180	NH1	ARG	198	19.689	30.115	35.005
	ATOM	1181	HH1	ARG	198	19.525	30.099	36.022
25	ATOM	1182	HH1	ARG	198	18.983	29.726	34.363
	ATOM	1183	NH2	ARG	198	21.769	31.166	35.363
	ATOM	1184	HH2	ARG	198	21.601	31.148	36.379
	ATOM	1185	HH2	ARG	198	22.640	31.573	34.993
	ATOM	1186	C	ARG	198	21.858	30.110	27.504
30	ATOM	1187	O	ARG	198	22.486	29.064	27.662
	ATOM	1188	N	TRP	199	22.055	30.935	26.454
	ATOM	1189	HN	TRP	199	21.571	31.844	26.462
	ATOM	1190	CA	TRP	199	22.892	30.634	25.328
	ATOM	1191	HA	TRP	199	22.572	29.703	24.859
35	ATOM	1192	CB	TRP	199	22.851	31.783	24.304
	ATOM	1193	HB1	TRP	199	23.539	32.556	24.649
	ATOM	1194	HB2	TRP	199	21.827	32.154	24.265
	ATOM	1195	CG	TRP	199	23.247	31.455	22.881
	ATOM	1196	CD2	TRP	199	24.577	31.186	22.406
40	ATOM	1197	CD1	TRP	199	22.425	31.352	21.798
	ATOM	1198	HD1	TRP	199	21.344	31.491	21.819
	ATOM	1199	NE1	TRP	199	23.156	31.046	20.677
	ATOM	1200	HE1	TRP	199	22.778	30.919	19.727
	ATOM	1201	CE2	TRP	199	24.481	30.936	21.036
45	ATOM	1202	CE3	TRP	199	25.778	31.148	23.055
	ATOM	1203	HE3	TRP	199	25.852	31.343	24.125
	ATOM	1204	CZ2	TRP	199	25.588	30.645	20.293
	ATOM	1205	HZ2	TRP	199	25.516	30.451	19.222
	ATOM	1206	CZ3	TRP	199	26.892	30.853	22.300
50	ATOM	1207	HZ3	TRP	199	27.869	30.813	22.783
	ATOM	1208	CH2	TRP	199	26.799	30.607	20.946
	ATOM	1209	HH2	TRP	199	27.703	30.377	20.382
	ATOM	1210	C	TRP	199	24.316	30.487	25.766
	ATOM	1211	O	TRP	199	24.886	29.398	25.718
55	ATOM	1212	N	GLN	200	24.919	31.599	26.223
	ATOM	1213	HN	GLN	200	24.369	32.466	26.302
	ATOM	1214	CA	GLN	200	26.301	31.616	26.604
	ATOM	1215	HA	GLN	200	26.890	31.084	25.856
	ATOM	1216	CB	GLN	200	26.879	33.034	26.774
60	ATOM	1217	HB1	GLN	200	27.898	32.945	27.148
	ATOM	1218	HB2	GLN	200	26.253	33.574	27.486
	ATOM	1219	CG	GLN	200	26.930	33.860	25.488
	ATOM	1220	HG1	GLN	200	27.298	33.211	24.693
	ATOM	1221	HG2	GLN	200	27.607	34.697	25.659
65	ATOM	1222	CD	GLN	200	25.520	34.344	25.193
	ATOM	1223	OE1	GLN	200	24.781	34.733	26.097
	ATOM	1224	NE2	GLN	200	25.128	34.314	23.891
	ATOM	1225	HE2	GLN	200	25.779	33.982	23.165

```
ATOM   1226  HE2 GLN   200      24.181  34.624  23.631
ATOM   1227  C   GLN   200      26.459  30.951  27.925
ATOM   1228  O   GLN   200      27.535  30.451  28.249
ATOM   1229  N   ASP   201      25.376  30.913  28.720
ATOM   1230  HN  ASP   201      24.449  31.176  28.356
ATOM   1231  CA  ASP   201      25.536  30.502  30.078
ATOM   1232  HA  ASP   201      26.193  31.165  30.641
ATOM   1233  CB  ASP   201      24.237  30.539  30.900
ATOM   1234  HB1 ASP   201      23.616  29.705  30.573
ATOM   1235  HB2 ASP   201      23.750  31.495  30.704
ATOM   1236  CG  ASP   201      24.617  30.403  32.372
ATOM   1237  OD1 ASP   201      25.173  29.339  32.757
ATOM   1238  OD2 ASP   201      24.369  31.378  33.131
ATOM   1239  C   ASP   201      26.123  29.134  30.197
ATOM   1240  O   ASP   201      27.102  28.967  30.921
ATOM   1241  N   ILE   202      25.603  28.107  29.498
ATOM   1242  HN  ILE   202      24.837  28.204  28.817
ATOM   1243  CA  ILE   202      26.241  26.862  29.814
ATOM   1244  HA  ILE   202      27.009  26.996  30.576
ATOM   1245  CB  ILE   202      25.355  25.809  30.414
ATOM   1246  HB  ILE   202      24.759  26.264  31.206
ATOM   1247  CG2 ILE   202      24.439  25.250  29.314
ATOM   1248  HG2 ILE   202      23.789  24.484  29.736
ATOM   1249  HG2 ILE   202      23.830  26.056  28.903
ATOM   1250  HG2 ILE   202      25.047  24.814  28.521
ATOM   1251  CG1 ILE   202      26.233  24.737  31.085
ATOM   1252  HG1 ILE   202      27.005  25.240  31.668
ATOM   1253  HG1 ILE   202      26.682  24.123  30.304
ATOM   1254  CD1 ILE   202      25.471  23.808  32.027
ATOM   1255  HD1 ILE   202      26.160  23.083  32.459
ATOM   1256  HD1 ILE   202      25.014  24.394  32.824
ATOM   1257  HD1 ILE   202      24.694  23.285  31.470
ATOM   1258  C   ILE   202      26.892  26.272  28.612
ATOM   1259  O   ILE   202      26.515  26.545  27.474
ATOM   1260  N   SER   203      27.907  25.428  28.878
ATOM   1261  HN  SER   203      28.135  25.234  29.863
ATOM   1262  CA  SER   203      28.683  24.788  27.864
ATOM   1263  HA  SER   203      28.104  24.825  26.941
ATOM   1264  CB  SER   203      30.043  25.464  27.606
ATOM   1265  HB1 SER   203      29.910  26.501  27.299
ATOM   1266  HB2 SER   203      30.591  24.947  26.818
ATOM   1267  OG  SER   203      30.845  25.453  28.778
ATOM   1268  HG  SER   203      31.198  26.403  28.963
ATOM   1269  C   SER   203      28.920  23.378  28.309
ATOM   1270  O   SER   203      27.984  22.666  28.667
ATOM   1271  N   MET   204      30.192  22.935  28.258
ATOM   1272  HN  MET   204      30.923  23.601  27.968
ATOM   1273  CA  MET   204      30.596  21.596  28.581
ATOM   1274  HA  MET   204      30.237  20.874  27.847
ATOM   1275  CB  MET   204      32.123  21.401  28.594
ATOM   1276  HB1 MET   204      32.609  21.685  27.661
ATOM   1277  HB2 MET   204      32.431  20.370  28.769
ATOM   1278  CG  MET   204      32.837  22.215  29.675
ATOM   1279  HG1 MET   204      32.415  21.941  30.642
ATOM   1280  HG2 MET   204      32.673  23.273  29.469
ATOM   1281  SD  MET   204      34.634  21.947  29.766
ATOM   1282  CE  MET   204      35.008  22.758  28.184
ATOM   1283  HE1 MET   204      36.082  22.725  28.004
ATOM   1284  HE2 MET   204      34.488  22.240  27.378
ATOM   1285  HE3 MET   204      34.678  23.796  28.221
ATOM   1286  C   MET   204      30.072  21.159  29.913
ATOM   1287  O   MET   204      29.383  21.886  30.629
ATOM   1288  N   MET   205      30.427  19.909  30.266
ATOM   1289  HN  MET   205      31.067  19.406  29.636
ATOM   1290  CA  MET   205      29.990  19.220  31.443
ATOM   1291  HA  MET   205      28.901  19.171  31.454
ATOM   1292  CB  MET   205      30.545  17.792  31.508
ATOM   1293  HB1 MET   205      31.619  17.849  31.686
```

ATOM	1294	HB2	MET	205	30.340	17.300	30.557
ATOM	1295	CG	MET	205	29.935	16.939	32.614
ATOM	1296	HG1	MET	205	28.856	16.814	32.517
ATOM	1297	HG2	MET	205	30.090	17.351	33.611
ATOM	1298	SD	MET	205	30.610	15.257	32.677
ATOM	1299	CE	MET	205	29.841	14.726	31.118
ATOM	1300	HE1	MET	205	30.107	13.689	30.916
ATOM	1301	HE2	MET	205	28.758	14.814	31.199
ATOM	1302	HE3	MET	205	30.197	15.358	30.304
ATOM	1303	C	MET	205	30.466	19.951	32.656
ATOM	1304	O	MET	205	29.792	19.953	33.685
ATOM	1305	N	ARG	206	31.649	20.582	32.573
ATOM	1306	HN	ARG	206	32.168	20.584	31.683
ATOM	1307	CA	ARG	206	32.193	21.253	33.719
ATOM	1308	HA	ARG	206	32.346	20.537	34.526
ATOM	1309	CB	ARG	206	33.535	21.941	33.423
ATOM	1310	HB1	ARG	206	33.476	22.671	32.616
ATOM	1311	HB2	ARG	206	34.320	21.245	33.127
ATOM	1312	CG	ARG	206	34.100	22.704	34.620
ATOM	1313	HG1	ARG	206	34.234	22.087	35.509
ATOM	1314	HG2	ARG	206	33.472	23.533	34.947
ATOM	1315	CD	ARG	206	35.472	23.326	34.361
ATOM	1316	HD1	ARG	206	35.729	23.910	35.245
ATOM	1317	HD2	ARG	206	35.375	23.954	33.475
ATOM	1318	NE	ARG	206	36.425	22.203	34.142
ATOM	1319	HE	ARG	206	36.707	21.939	33.187
ATOM	1320	CZ	ARG	206	36.922	21.524	35.218
ATOM	1321	NH1	ARG	206	36.524	21.865	36.479
ATOM	1322	HH1	ARG	206	36.898	21.355	37.292
ATOM	1323	HH1	ARG	206	35.851	22.632	36.617
ATOM	1324	NH2	ARG	206	37.806	20.501	35.032
ATOM	1325	HH2	ARG	206	38.181	19.990	35.844
ATOM	1326	HH2	ARG	206	38.099	20.240	34.080
ATOM	1327	C	ARG	206	31.245	22.317	34.177
ATOM	1328	O	ARG	206	30.931	22.407	35.363
ATOM	1329	N	MET	207	30.745	23.148	33.245
ATOM	1330	HN	MET	207	30.992	23.020	32.253
ATOM	1331	CA	MET	207	29.868	24.212	33.636
ATOM	1332	HA	MET	207	30.358	24.805	34.407
ATOM	1333	CB	MET	207	29.527	25.178	32.487
ATOM	1334	HB1	MET	207	28.776	25.915	32.771
ATOM	1335	HB2	MET	207	29.134	24.663	31.611
ATOM	1336	CG	MET	207	30.747	25.971	32.007
ATOM	1337	HG1	MET	207	31.400	25.291	31.460
ATOM	1338	HG2	MET	207	31.255	26.375	32.883
ATOM	1339	SD	MET	207	30.371	27.368	30.905
ATOM	1340	CE	MET	207	29.718	28.430	32.219
ATOM	1341	HE1	MET	207	29.405	29.384	31.795
ATOM	1342	HE2	MET	207	28.863	27.944	32.689
ATOM	1343	HE3	MET	207	30.493	28.603	32.966
ATOM	1344	C	MET	207	28.604	23.622	34.165
ATOM	1345	O	MET	207	28.017	24.138	35.113
ATOM	1346	N	LYS	208	28.162	22.503	33.568
ATOM	1347	HN	LYS	208	28.721	22.081	32.812
ATOM	1348	CA	LYS	208	26.932	21.883	33.959
ATOM	1349	HA	LYS	208	26.113	22.595	33.857
ATOM	1350	CB	LYS	208	26.588	20.656	33.100
ATOM	1351	HB1	LYS	208	25.687	20.147	33.445
ATOM	1352	HB2	LYS	208	27.383	19.910	33.104
ATOM	1353	CG	LYS	208	26.344	21.019	31.636
ATOM	1354	HG1	LYS	208	27.155	21.666	31.304
ATOM	1355	HG2	LYS	208	25.387	21.537	31.566
ATOM	1356	CD	LYS	208	26.292	19.818	30.696
ATOM	1357	HD1	LYS	208	25.447	19.160	30.896
ATOM	1358	HD2	LYS	208	27.181	19.190	30.762
ATOM	1359	CE	LYS	208	26.171	20.221	29.224
ATOM	1360	HE1	LYS	208	26.057	19.330	28.606
ATOM	1361	HE2	LYS	208	27.067	20.759	28.914

ATOM	1362	NZ	LYS	208	24.991	21.095	29.040
ATOM	1363	HZ1	LYS	208	24.913	21.363	28.049
ATOM	1364	HZ2	LYS	208	24.140	20.588	29.326
ATOM	1365	HZ3	LYS	208	25.096	21.941	29.617
ATOM	1366	C	LYS	208	27.021	21.436	35.384
ATOM	1367	O	LYS	208	26.035	21.468	36.113
ATOM	1368	N	THR	209	28.203	20.970	35.808
ATOM	1369	HN	THR	209	28.996	20.971	35.150
ATOM	1370	CA	THR	209	28.418	20.469	37.137
ATOM	1371	HA	THR	209	27.630	19.795	37.471
ATOM	1372	CB	THR	209	29.652	19.629	37.255
ATOM	1373	HB	THR	209	29.702	19.268	38.283
ATOM	1374	OG1	THR	209	30.816	20.390	36.970
ATOM	1375	HG1	THR	209	31.573	20.116	37.613
ATOM	1376	CG2	THR	209	29.514	18.469	36.258
ATOM	1377	HG2	THR	209	30.397	17.832	36.315
ATOM	1378	HG2	THR	209	28.628	17.883	36.502
ATOM	1379	HG2	THR	209	29.418	18.867	35.247
ATOM	1380	C	THR	209	28.488	21.556	38.171
ATOM	1381	O	THR	209	28.309	21.281	39.357
ATOM	1382	N	ILE	210	28.765	22.811	37.770
ATOM	1383	HN	ILE	210	28.804	23.026	36.763
ATOM	1384	CA	ILE	210	29.007	23.858	38.729
ATOM	1385	HA	ILE	210	29.899	23.675	39.327
ATOM	1386	CB	ILE	210	29.261	25.197	38.087
ATOM	1387	HB	ILE	210	30.064	25.093	37.357
ATOM	1388	CG2	ILE	210	27.975	25.670	37.390
ATOM	1389	HG2	ILE	210	28.150	26.639	36.923
ATOM	1390	HG2	ILE	210	27.687	24.946	36.628
ATOM	1391	HG2	ILE	210	27.175	25.760	38.125
ATOM	1392	CG1	ILE	210	29.803	26.193	39.125
ATOM	1393	HG1	ILE	210	30.619	25.792	39.726
ATOM	1394	HG1	ILE	210	29.051	26.521	39.844
ATOM	1395	CD1	ILE	210	30.353	27.477	38.506
ATOM	1396	HD1	ILE	210	30.718	28.134	39.295
ATOM	1397	HD1	ILE	210	31.172	27.232	37.830
ATOM	1398	HD1	ILE	210	29.562	27.981	37.950
ATOM	1399	C	ILE	210	27.869	24.019	39.700
ATOM	1400	O	ILE	210	28.106	24.125	40.902
ATOM	1401	N	GLY	211	26.602	24.043	39.245
ATOM	1402	HN	GLY	211	26.394	23.941	38.241
ATOM	1403	CA	GLY	211	25.549	24.214	40.210
ATOM	1404	HA1	GLY	211	25.282	25.271	40.211
ATOM	1405	HA2	GLY	211	25.942	23.898	41.176
ATOM	1406	C	GLY	211	24.410	23.362	39.775
ATOM	1407	O	GLY	211	24.440	22.797	38.684
ATOM	1408	N	GLU	212	23.383	23.205	40.640
ATOM	1409	HN	GLU	212	23.387	23.626	41.580
ATOM	1410	CA	GLU	212	22.293	22.415	40.163
ATOM	1411	HA	GLU	212	22.642	21.508	39.670
ATOM	1412	CB	GLU	212	21.156	22.073	41.138
ATOM	1413	HB1	GLU	212	20.767	22.954	41.647
ATOM	1414	HB2	GLU	212	21.474	21.381	41.918
ATOM	1415	CG	GLU	212	19.962	21.415	40.433
ATOM	1416	HG1	GLU	212	19.930	21.726	39.389
ATOM	1417	HG2	GLU	212	19.034	21.712	40.921
ATOM	1418	CD	GLU	212	20.093	19.903	40.496
ATOM	1419	OE1	GLU	212	19.844	19.346	41.597
ATOM	1420	OE2	GLU	212	20.420	19.287	39.448
ATOM	1422	C	GLU	212	21.640	23.352	39.227
ATOM	1423	O	GLU	212	21.015	24.313	39.669
ATOM	1424	N	HIS	213	21.775	23.098	37.916
ATOM	1425	HN	HIS	213	22.243	22.235	37.604
ATOM	1426	CA	HIS	213	21.272	24.025	36.956
ATOM	1427	HA	HIS	213	21.693	25.019	37.105
ATOM	1428	ND1	HIS	213	24.202	23.591	35.496
ATOM	1429	HD1	HIS	213	24.304	22.682	35.970
ATOM	1430	CG	HIS	213	23.024	24.223	35.174

ATOM	1431	NE2	HIS	213	24.756	25.499	34.494
ATOM	1432	HE2	HIS	213	25.306	26.269	34.088
ATOM	1433	CD2	HIS	213	23.379	25.385	34.561
ATOM	1434	HD2	HIS	213	22.676	26.124	34.176
ATOM	1435	CE1	HIS	213	25.206	24.398	35.067
ATOM	1436	HE1	HIS	213	26.264	24.163	35.182
ATOM	1437	CB	HIS	213	21.659	23.701	35.503
ATOM	1438	HB1	HIS	213	20.957	24.146	34.797
ATOM	1439	HB2	HIS	213	21.666	22.625	35.326
ATOM	1440	C	HIS	213	19.789	24.147	37.046
ATOM	1441	O	HIS	213	19.267	25.255	36.949
ATOM	1442	N	ILE	214	19.068	23.031	37.257
ATOM	1443	HN	ILE	214	19.548	22.130	37.389
ATOM	1444	CA	ILE	214	17.634	23.088	37.302
ATOM	1445	HA	ILE	214	17.275	23.468	36.345
ATOM	1446	CB	ILE	214	17.022	21.728	37.528
ATOM	1447	HB	ILE	214	17.416	21.055	36.767
ATOM	1448	CG2	ILE	214	17.420	21.263	38.937
ATOM	1449	HG2	ILE	214	16.991	20.280	39.131
ATOM	1450	HG2	ILE	214	18.506	21.206	39.008
ATOM	1451	HG2	ILE	214	17.045	21.974	39.674
ATOM	1452	CG1	ILE	214	15.503	21.722	37.266
ATOM	1453	HG1	ILE	214	15.152	20.692	37.326
ATOM	1454	HG1	ILE	214	15.328	22.132	36.272
ATOM	1455	CD1	ILE	214	14.677	22.546	38.254
ATOM	1456	HD1	ILE	214	13.622	22.481	37.990
ATOM	1457	HD1	ILE	214	14.823	22.158	39.262
ATOM	1458	HD1	ILE	214	14.997	23.587	38.216
ATOM	1459	C	ILE	214	17.231	24.007	38.418
ATOM	1460	O	ILE	214	16.278	24.771	38.272
ATOM	1461	N	VAL	215	17.948	23.970	39.561
ATOM	1462	HN	VAL	215	18.754	23.333	39.636
ATOM	1463	CA	VAL	215	17.599	24.812	40.677
ATOM	1464	HA	VAL	215	16.578	24.580	40.981
ATOM	1465	CB	VAL	215	18.573	24.769	41.818
ATOM	1466	HB	VAL	215	19.552	25.061	41.437
ATOM	1467	CG1	VAL	215	18.088	25.753	42.894
ATOM	1468	HG1	VAL	215	18.779	25.741	43.736
ATOM	1469	HG1	VAL	215	18.044	26.758	42.474
ATOM	1470	HG1	VAL	215	17.095	25.459	43.235
ATOM	1471	CG2	VAL	215	18.762	23.337	42.309
ATOM	1472	HG2	VAL	215	19.472	23.327	43.136
ATOM	1473	HG2	VAL	215	17.806	22.939	42.646
ATOM	1474	HG2	VAL	215	19.145	22.721	41.495
ATOM	1475	C	VAL	215	17.701	26.234	40.249
ATOM	1476	O	VAL	215	16.816	27.039	40.530
ATOM	1477	N	ALA	216	18.811	26.581	39.575
ATOM	1478	HN	ALA	216	19.505	25.863	39.324
ATOM	1479	CA	ALA	216	19.031	27.946	39.204
ATOM	1480	HA	ALA	216	18.971	28.588	40.083
ATOM	1481	CB	ALA	216	20.420	28.184	38.591
ATOM	1482	HB1	ALA	216	20.527	29.237	38.331
ATOM	1483	HB2	ALA	216	21.189	27.909	39.314
ATOM	1484	HB3	ALA	216	20.531	27.576	37.694
ATOM	1485	C	ALA	216	17.993	28.387	38.213
ATOM	1486	O	ALA	216	17.436	29.478	38.331
ATOM	1487	N	HIS	217	17.693	27.533	37.217
ATOM	1488	HN	HIS	217	18.138	26.605	37.208
ATOM	1489	CA	HIS	217	16.774	27.870	36.166
ATOM	1490	HA	HIS	217	17.111	28.781	35.671
ATOM	1491	ND1	HIS	217	18.889	27.082	34.036
ATOM	1492	HD1	HIS	217	18.875	28.112	34.020
ATOM	1493	CG	HIS	217	17.908	26.255	34.537
ATOM	1494	NE2	HIS	217	19.599	24.996	33.731
ATOM	1495	HE2	HIS	217	20.177	24.187	33.465
ATOM	1496	CD2	HIS	217	18.357	24.985	34.341
ATOM	1497	HD2	HIS	217	17.813	24.084	34.625
ATOM	1498	CE1	HIS	217	19.877	26.277	33.568

```
ATOM   1499  HE1 HIS   217      20.794  26.646  33.109
ATOM   1500  CB  HIS   217      16.620  26.727  35.147
ATOM   1501  HB1 HIS   217      15.982  27.078  34.336
ATOM   1502  HB2 HIS   217      16.165  25.876  35.654
ATOM   1503  C   HIS   217      15.415  28.088  36.749
ATOM   1504  O   HIS   217      14.711  29.038  36.403
ATOM   1505  N   ILE   218      15.017  27.190  37.662
ATOM   1506  HN  ILE   218      15.676  26.451  37.947
ATOM   1507  CA  ILE   218      13.717  27.215  38.255
ATOM   1508  HA  ILE   218      12.960  27.231  37.471
ATOM   1509  CB  ILE   218      13.447  25.975  39.062
ATOM   1510  HB  ILE   218      13.729  25.100  38.477
ATOM   1511  CG2 ILE   218      14.273  26.027  40.355
ATOM   1512  HG2 ILE   218      14.082  25.131  40.946
ATOM   1513  HG2 ILE   218      15.333  26.079  40.108
ATOM   1514  HG2 ILE   218      13.992  26.908  40.932
ATOM   1515  CG1 ILE   218      11.943  25.805  39.298
ATOM   1516  HG1 ILE   218      11.352  26.002  38.404
ATOM   1517  HG1 ILE   218      11.560  26.476  40.067
ATOM   1518  CD1 ILE   218      11.573  24.394  39.747
ATOM   1519  HD1 ILE   218      10.495  24.331  39.900
ATOM   1520  HD1 ILE   218      11.873  23.678  38.982
ATOM   1521  HD1 ILE   218      12.085  24.163  40.681
ATOM   1522  C   ILE   218      13.579  28.438  39.107
ATOM   1523  O   ILE   218      12.496  29.013  39.207
ATOM   1524  N   GLN   219      14.684  28.884  39.733
ATOM   1525  HN  GLN   219      15.580  28.394  39.604
ATOM   1526  CA  GLN   219      14.618  30.040  40.581
ATOM   1527  HA  GLN   219      13.921  29.807  41.386
ATOM   1528  CB  GLN   219      15.987  30.457  41.145
ATOM   1529  HB1 GLN   219      15.858  31.377  41.715
ATOM   1530  HB2 GLN   219      16.668  30.617  40.309
ATOM   1531  CG  GLN   219      16.621  29.419  42.072
ATOM   1532  HG1 GLN   219      16.751  28.501  41.498
ATOM   1533  HG2 GLN   219      15.942  29.269  42.911
ATOM   1534  CD  GLN   219      17.961  29.975  42.536
ATOM   1535  OE1 GLN   219      19.007  29.358  42.344
ATOM   1536  NE2 GLN   219      17.928  31.177  43.175
ATOM   1537  HE2 GLN   219      17.030  31.660  43.316
ATOM   1538  HE2 GLN   219      18.801  31.602  43.517
ATOM   1539  C   GLN   219      14.132  31.173  39.740
ATOM   1540  O   GLN   219      13.303  31.969  40.178
ATOM   1541  N   HIS   220      14.627  31.261  38.493
ATOM   1542  HN  HIS   220      15.305  30.562  38.157
ATOM   1543  CA  HIS   220      14.212  32.327  37.632
ATOM   1544  HA  HIS   220      14.492  33.265  38.111
ATOM   1545  ND1 HIS   220      17.279  31.761  36.687
ATOM   1546  HD1 HIS   220      17.157  30.847  37.146
ATOM   1547  CG  HIS   220      16.283  32.567  36.183
ATOM   1548  NE2 HIS   220      18.280  33.562  35.850
ATOM   1549  HE2 HIS   220      19.002  34.239  35.567
ATOM   1550  CD2 HIS   220      16.912  33.660  35.676
ATOM   1551  HD2 HIS   220      16.407  34.499  35.197
ATOM   1552  CE1 HIS   220      18.452  32.404  36.462
ATOM   1553  HE1 HIS   220      19.426  32.010  36.752
ATOM   1554  CB  HIS   220      14.821  32.237  36.222
ATOM   1555  HB1 HIS   220      14.355  32.913  35.505
ATOM   1556  HB2 HIS   220      14.739  31.245  35.777
ATOM   1557  C   HIS   220      12.731  32.222  37.468
ATOM   1558  O   HIS   220      12.014  33.218  37.543
ATOM   1559  N   GLU   221      12.237  30.991  37.255
ATOM   1560  HN  GLU   221      12.881  30.187  37.231
ATOM   1561  CA  GLU   221      10.835  30.772  37.058
ATOM   1562  HA  GLU   221      10.492  31.344  36.197
ATOM   1563  CB  GLU   221      10.519  29.283  36.819
ATOM   1564  HB1 GLU   221      11.098  28.692  37.529
ATOM   1565  HB2 GLU   221      10.800  29.035  35.795
ATOM   1566  CG  GLU   221       9.046  28.913  36.999
```

ATOM	1567	HG1	GLU	221	8.822	28.111	36.295
ATOM	1568	HG2	GLU	221	8.457	29.805	36.786
ATOM	1569	CD	GLU	221	8.863	28.455	38.442
ATOM	1570	OE1	GLU	221	9.899	28.242	39.126
ATOM	1571	OE2	GLU	221	7.690	28.302	38.875
ATOM	1573	C	GLU	221	10.082	31.210	38.275
ATOM	1574	O	GLU	221	9.118	31.968	38.179
ATOM	1575	N	VAL	222	10.550	30.761	39.453
ATOM	1576	HN	VAL	222	11.389	30.164	39.425
ATOM	1577	CA	VAL	222	9.989	31.036	40.745
ATOM	1578	HA	VAL	222	10.193	30.260	41.482
ATOM	1579	CB	VAL	222	10.606	32.242	41.403
ATOM	1580	HB	VAL	222	11.666	32.056	41.575
ATOM	1581	CG1	VAL	222	10.439	33.466	40.485
ATOM	1582	HG1	VAL	222	10.885	34.340	40.959
ATOM	1583	HG1	VAL	222	10.935	33.277	39.533
ATOM	1584	HG1	VAL	222	9.378	33.648	40.312
ATOM	1585	CG2	VAL	222	9.978	32.417	42.796
ATOM	1586	HG2	VAL	222	10.415	33.287	43.286
ATOM	1587	HG2	VAL	222	8.902	32.560	42.695
ATOM	1588	HG2	VAL	222	10.170	31.527	43.396
ATOM	1589	C	VAL	222	8.495	31.179	40.730
ATOM	1590	O	VAL	222	7.982	32.255	40.437
ATOM	1591	N	ASP	223	7.777	30.070	41.055
ATOM	1592	HN	ASP	223	8.297	29.192	41.194
ATOM	1593	CA	ASP	223	6.339	30.030	41.221
ATOM	1594	HA	ASP	223	6.009	30.612	42.082
ATOM	1595	CB	ASP	223	5.484	30.685	40.115
ATOM	1596	HB1	ASP	223	4.538	30.147	40.060
ATOM	1597	HB2	ASP	223	6.033	30.606	39.177
ATOM	1598	CG	ASP	223	5.261	32.145	40.496
ATOM	1599	OD1	ASP	223	5.616	32.509	41.650
ATOM	1600	OD2	ASP	223	4.737	32.913	39.646
ATOM	1601	C	ASP	223	5.830	28.624	41.427
ATOM	1602	O	ASP	223	6.563	27.742	41.868
ATOM	1603	N	PHE	224	4.523	28.411	41.120
ATOM	1604	HN	PHE	224	4.000	29.205	40.723
ATOM	1605	CA	PHE	224	3.801	27.176	41.300
ATOM	1606	HA	PHE	224	3.677	26.937	42.356
ATOM	1607	CB	PHE	224	2.382	27.181	40.693
ATOM	1608	HB1	PHE	224	2.020	26.162	40.558
ATOM	1609	HB2	PHE	224	2.383	27.676	39.722
ATOM	1610	CG	PHE	224	1.432	27.903	41.589
ATOM	1611	CD1	PHE	224	1.441	29.275	41.686
ATOM	1612	HD1	PHE	224	2.157	29.854	41.103
ATOM	1613	CD2	PHE	224	0.503	27.192	42.315
ATOM	1614	HD2	PHE	224	0.474	26.106	42.232
ATOM	1615	CE1	PHE	224	0.552	29.923	42.514
ATOM	1616	HE1	PHE	224	0.574	31.010	42.590
ATOM	1617	CE2	PHE	224	-0.386	27.833	43.142
ATOM	1618	HE2	PHE	224	-1.112	27.256	43.716
ATOM	1619	CZ	PHE	224	-0.361	29.203	43.245
ATOM	1620	HZ	PHE	224	-1.062	29.716	43.902
ATOM	1621	C	PHE	224	4.517	26.027	40.662
ATOM	1622	O	PHE	224	5.617	26.154	40.129
ATOM	1623	N	LEU	225	3.841	24.859	40.720
ATOM	1624	HN	LEU	225	2.918	24.898	41.175
ATOM	1625	CA	LEU	225	4.243	23.569	40.227
ATOM	1626	HA	LEU	225	4.881	23.079	40.963
ATOM	1627	CB	LEU	225	2.995	22.680	39.996
ATOM	1628	HB1	LEU	225	2.360	23.201	39.279
ATOM	1629	HB2	LEU	225	2.502	22.561	40.960
ATOM	1630	CG	LEU	225	3.186	21.253	39.437
ATOM	1631	HG	LEU	225	3.913	20.712	40.041
ATOM	1632	CD2	LEU	225	3.772	21.234	38.017
ATOM	1633	HD2	LEU	225	3.881	20.202	37.682
ATOM	1634	HD2	LEU	225	3.104	21.766	37.340
ATOM	1635	HD2	LEU	225	4.748	21.719	38.020

ATOM	1636	CD1	LEU	225	1.850	20.498	39.467
ATOM	1637	HD1	LEU	225	1.992	19.492	39.071
ATOM	1638	HD1	LEU	225	1.490	20.436	40.493
ATOM	1639	HD1	LEU	225	1.119	21.028	38.856
ATOM	1640	C	LEU	225	5.000	23.732	38.948
ATOM	1641	O	LEU	225	4.719	24.655	38.187
ATOM	1642	N	PHE	226	5.995	22.840	38.693
ATOM	1643	HN	PHE	226	6.207	22.104	39.381
ATOM	1644	CA	PHE	226	6.755	22.913	37.471
ATOM	1645	HA	PHE	226	6.249	23.571	36.764
ATOM	1646	CB	PHE	226	8.153	23.549	37.608
ATOM	1647	HB1	PHE	226	8.092	24.525	38.090
ATOM	1648	HB2	PHE	226	8.616	23.685	36.630
ATOM	1649	CG	PHE	226	9.049	22.690	38.423
ATOM	1650	CD1	PHE	226	9.081	22.819	39.790
ATOM	1651	HD1	PHE	226	8.440	23.552	40.281
ATOM	1652	CD2	PHE	226	9.861	21.759	37.817
ATOM	1653	HD2	PHE	226	9.839	21.648	36.733
ATOM	1654	CE1	PHE	226	9.915	22.030	40.540
ATOM	1655	HE1	PHE	226	9.934	22.138	41.625
ATOM	1656	CE2	PHE	226	10.698	20.968	38.565
ATOM	1657	HE2	PHE	226	11.338	20.234	38.076
ATOM	1658	CZ	PHE	226	10.727	21.105	39.932
ATOM	1659	HZ	PHE	226	11.392	20.482	40.530
ATOM	1660	C	PHE	226	6.880	21.538	36.870
ATOM	1661	O	PHE	226	6.370	20.561	37.417
ATOM	1662	N	CYS	227	7.563	21.439	35.704
ATOM	1663	HN	CYS	227	8.072	22.263	35.352
ATOM	1664	CA	CYS	227	7.600	20.217	34.941
ATOM	1665	HA	CYS	227	7.270	19.370	35.542
ATOM	1666	CB	CYS	227	6.745	20.338	33.681
ATOM	1667	HB1	CYS	227	5.700	20.434	33.976
ATOM	1668	HB2	CYS	227	6.885	19.442	33.076
ATOM	1669	SG	CYS	227	7.273	21.807	32.758
ATOM	1670	HG	CYS	227	8.271	22.414	33.416
ATOM	1671	C	CYS	227	8.994	19.924	34.456
ATOM	1672	O	CYS	227	9.930	20.685	34.696
ATOM	1673	N	MET	228	9.138	18.775	33.746
ATOM	1674	HN	MET	228	8.300	18.195	33.598
ATOM	1675	CA	MET	228	10.384	18.311	33.183
ATOM	1676	HA	MET	228	11.162	19.057	33.351
ATOM	1677	CB	MET	228	10.920	16.997	33.783
ATOM	1678	HB1	MET	228	11.690	16.604	33.119
ATOM	1679	HB2	MET	228	10.092	16.294	33.866
ATOM	1680	CG	MET	228	11.539	17.159	35.175
ATOM	1681	HG1	MET	228	10.767	17.527	35.850
ATOM	1682	HG2	MET	228	12.360	17.872	35.102
ATOM	1683	SD	MET	228	12.208	15.627	35.891
ATOM	1684	CE	MET	228	13.052	16.449	37.274
ATOM	1685	HE1	MET	228	13.557	15.702	37.887
ATOM	1686	HE2	MET	228	13.785	17.155	36.885
ATOM	1687	HE3	MET	228	12.321	16.982	37.881
ATOM	1688	C	MET	228	10.219	18.088	31.698
ATOM	1689	O	MET	228	9.166	18.384	31.135
ATOM	1690	N	ASP	229	11.276	17.543	31.040
ATOM	1691	HN	ASP	229	12.046	17.175	31.617
ATOM	1692	CA	ASP	229	11.419	17.432	29.599
ATOM	1693	HA	ASP	229	11.556	18.408	29.134
ATOM	1694	CB	ASP	229	12.584	16.502	29.221
ATOM	1695	HB1	ASP	229	12.660	16.448	28.135
ATOM	1696	HB2	ASP	229	12.396	15.509	29.628
ATOM	1697	CG	ASP	229	13.877	17.061	29.800
ATOM	1698	OD1	ASP	229	14.290	18.175	29.383
ATOM	1699	OD2	ASP	229	14.473	16.367	30.667
ATOM	1700	C	ASP	229	10.209	16.804	28.972
ATOM	1701	O	ASP	229	9.504	17.462	28.217
ATOM	1702	N	VAL	230	9.990	15.496	29.198
ATOM	1703	HN	VAL	230	10.766	14.939	29.583

ATOM	1704	CA	VAL	230	8.745	14.819	28.939
ATOM	1705	HA	VAL	230	7.900	15.498	28.819
ATOM	1706	CB	VAL	230	8.738	13.658	27.992
ATOM	1707	HB	VAL	230	9.299	13.902	27.090
ATOM	1708	CG1	VAL	230	9.384	12.421	28.656
ATOM	1709	HG1	VAL	230	9.372	11.585	27.957
ATOM	1710	HG1	VAL	230	10.414	12.651	28.929
ATOM	1711	HG1	VAL	230	8.822	12.154	29.551
ATOM	1712	CG2	VAL	230	7.280	13.400	27.600
ATOM	1713	HG2	VAL	230	7.232	12.558	26.909
ATOM	1714	HG2	VAL	230	6.698	13.169	28.493
ATOM	1715	HG2	VAL	230	6.869	14.288	27.120
ATOM	1716	C	VAL	230	8.776	14.078	30.176
ATOM	1717	O	VAL	230	7.814	13.442	30.614
ATOM	1718	N	ASP	231	9.954	14.330	30.781
ATOM	1719	HN	ASP	231	10.552	15.057	30.363
ATOM	1720	CA	ASP	231	10.438	13.684	31.933
ATOM	1721	HA	ASP	231	10.691	12.643	31.733
ATOM	1722	CB	ASP	231	11.666	14.402	32.516
ATOM	1723	HB1	ASP	231	11.345	15.332	32.986
ATOM	1724	HB2	ASP	231	12.368	14.617	31.709
ATOM	1725	CG	ASP	231	12.324	13.501	33.548
ATOM	1726	OD1	ASP	231	11.583	12.764	34.249
ATOM	1727	OD2	ASP	231	13.580	13.531	33.641
ATOM	1728	C	ASP	231	9.293	13.822	32.841
ATOM	1729	O	ASP	231	8.864	12.864	33.471
ATOM	1730	N	GLN	232	8.694	15.019	32.834
ATOM	1731	HN	GLN	232	9.097	15.815	32.320
ATOM	1732	CA	GLN	232	7.483	15.146	33.562
ATOM	1733	HA	GLN	232	7.365	14.212	34.112
ATOM	1734	CB	GLN	232	7.467	16.343	34.525
ATOM	1735	HB1	GLN	232	7.655	17.296	34.030
ATOM	1736	HB2	GLN	232	8.218	16.273	35.312
ATOM	1737	CG	GLN	232	6.135	16.517	35.249
ATOM	1738	HG1	GLN	232	5.387	16.788	34.503
ATOM	1739	HG2	GLN	232	6.261	17.309	35.987
ATOM	1740	CD	GLN	232	5.797	15.195	35.913
ATOM	1741	OE1	GLN	232	6.666	14.480	36.411
ATOM	1742	NE2	GLN	232	4.482	14.852	35.907
ATOM	1743	HE2	GLN	232	3.788	15.482	35.479
ATOM	1744	HE2	GLN	232	4.180	13.963	36.330
ATOM	1745	C	GLN	232	6.416	15.354	32.546
ATOM	1746	O	GLN	232	6.600	16.091	31.582
ATOM	1747	N	VAL	233	5.289	14.641	32.697
ATOM	1748	HN	VAL	233	5.217	13.926	33.435
ATOM	1749	CA	VAL	233	4.189	14.887	31.817
ATOM	1750	HA	VAL	233	4.381	15.867	31.380
ATOM	1751	CB	VAL	233	4.004	13.876	30.725
ATOM	1752	HB	VAL	233	3.104	14.130	30.165
ATOM	1753	CG1	VAL	233	5.233	13.915	29.805
ATOM	1754	HG1	VAL	233	5.112	13.185	29.005
ATOM	1755	HG1	VAL	233	5.334	14.911	29.374
ATOM	1756	HG1	VAL	233	6.127	13.677	30.381
ATOM	1757	CG2	VAL	233	3.736	12.511	31.360
ATOM	1758	HG2	VAL	233	3.599	11.766	30.576
ATOM	1759	HG2	VAL	233	4.583	12.228	31.985
ATOM	1760	HG2	VAL	233	2.835	12.564	31.971
ATOM	1761	C	VAL	233	2.981	14.859	32.678
ATOM	1762	O	VAL	233	2.931	14.124	33.664
ATOM	1763	N	PHE	234	1.973	15.682	32.341
ATOM	1764	HN	PHE	234	2.042	16.309	31.527
ATOM	1765	CA	PHE	234	0.804	15.652	33.158
ATOM	1766	HA	PHE	234	1.148	15.887	34.165
ATOM	1767	CB	PHE	234	-0.280	16.652	32.721
ATOM	1768	HB1	PHE	234	-1.159	16.444	33.331
ATOM	1769	HB2	PHE	234	-0.462	16.472	31.662
ATOM	1770	CG	PHE	234	0.269	18.014	32.974
ATOM	1771	CD1	PHE	234	0.224	18.559	34.237

```
ATOM   1772  HD1 PHE   234      -0.217  17.989  35.053
ATOM   1773  CD2 PHE   234       0.831  18.746  31.953
ATOM   1774  HD2 PHE   234       0.874  18.328  30.948
ATOM   1775  CE1 PHE   234       0.730  19.814  34.481
ATOM   1776  HE1 PHE   234       0.687  20.233  35.486
ATOM   1777  CE2 PHE   234       1.339  20.001  32.194
ATOM   1778  HE2 PHE   234       1.783  20.573  31.379
ATOM   1779  CZ  PHE   234       1.290  20.537  33.458
ATOM   1780  HZ  PHE   234       1.692  21.532  33.647
ATOM   1781  C   PHE   234       0.268  14.272  33.029
ATOM   1782  O   PHE   234      -0.201  13.878  31.963
ATOM   1783  N   GLN   235       0.341  13.500  34.131
ATOM   1784  HN  GLN   235       0.723  13.894  35.002
ATOM   1785  CA  GLN   235      -0.104  12.141  34.108
ATOM   1786  HA  GLN   235       0.356  11.676  33.236
ATOM   1787  CB  GLN   235       0.320  11.345  35.362
ATOM   1788  HB1 GLN   235      -0.228  11.744  36.215
ATOM   1789  HB2 GLN   235       1.394  11.474  35.494
ATOM   1790  CG  GLN   235       0.048   9.835  35.315
ATOM   1791  HG1 GLN   235      -1.024   9.672  35.212
ATOM   1792  HG2 GLN   235       0.407   9.382  36.238
ATOM   1793  CD  GLN   235       0.781   9.239  34.123
ATOM   1794  OE1 GLN   235       0.699   9.751  33.008
ATOM   1795  NE2 GLN   235       1.523   8.123  34.359
ATOM   1796  HE2 GLN   235       1.566   7.725  35.308
ATOM   1797  HE2 GLN   235       2.042   7.678  33.590
ATOM   1798  C   GLN   235      -1.590  12.182  34.004
ATOM   1799  O   GLN   235      -2.166  13.229  33.719
ATOM   1800  N   ASP   236      -2.248  11.029  34.224
ATOM   1801  HN  ASP   236      -1.726  10.189  34.511
ATOM   1802  CA  ASP   236      -3.662  10.965  34.061
ATOM   1803  HA  ASP   236      -3.938  10.002  34.490
ATOM   1804  CB  ASP   236      -4.442  12.107  34.741
ATOM   1805  HB1 ASP   236      -4.126  13.054  34.302
ATOM   1806  HB2 ASP   236      -4.222  12.092  35.808
ATOM   1807  CG  ASP   236      -5.932  11.886  34.504
ATOM   1808  OD1 ASP   236      -6.292  10.869  33.855
ATOM   1809  OD2 ASP   236      -6.733  12.735  34.978
ATOM   1810  C   ASP   236      -3.866  11.057  32.595
ATOM   1811  O   ASP   236      -3.893  10.045  31.898
ATOM   1812  N   LYS   237      -3.989  12.297  32.086
ATOM   1813  HN  LYS   237      -3.917  13.125  32.693
ATOM   1814  CA  LYS   237      -4.221  12.436  30.689
ATOM   1815  HA  LYS   237      -3.492  11.808  30.175
ATOM   1816  CB  LYS   237      -5.666  12.122  30.258
ATOM   1817  HB1 LYS   237      -5.765  12.380  29.204
ATOM   1818  HB2 LYS   237      -6.337  12.723  30.872
ATOM   1819  CG  LYS   237      -6.105  10.664  30.407
ATOM   1820  HG1 LYS   237      -5.839  10.240  31.374
ATOM   1821  HG2 LYS   237      -5.658  10.010  29.659
ATOM   1822  CD  LYS   237      -7.619  10.484  30.271
ATOM   1823  HD1 LYS   237      -7.920  10.835  29.284
ATOM   1824  HD2 LYS   237      -8.106  11.071  31.050
ATOM   1825  CE  LYS   237      -8.087   9.037  30.415
ATOM   1826  HE1 LYS   237      -7.810   8.655  31.398
ATOM   1827  HE2 LYS   237      -7.621   8.419  29.648
ATOM   1828  NZ  LYS   237      -9.558   8.967  30.266
ATOM   1829  HZ1 LYS   237      -9.868   7.990  30.364
ATOM   1830  HZ2 LYS   237     -10.005   9.544  30.993
ATOM   1831  HZ3 LYS   237      -9.826   9.321  29.336
ATOM   1832  C   LYS   237      -4.039  13.867  30.352
ATOM   1833  O   LYS   237      -2.991  14.465  30.588
ATOM   1834  N   PHE   238      -5.131  14.451  29.836
ATOM   1835  HN  PHE   238      -5.999  13.898  29.784
ATOM   1836  CA  PHE   238      -5.162  15.792  29.356
ATOM   1837  HA  PHE   238      -4.502  15.808  28.488
ATOM   1838  CB  PHE   238      -6.588  16.254  29.014
ATOM   1839  HB1 PHE   238      -6.516  17.282  28.660
```

```
ATOM   1840  HB2 PHE   238      -7.176  16.182  29.928
ATOM   1841  CG  PHE   238      -7.102  15.340  27.953
ATOM   1842  CD1 PHE   238      -6.804  15.553  26.628
ATOM   1843  HD1 PHE   238      -6.181  16.401  26.343
ATOM   1844  CD2 PHE   238      -7.889  14.263  28.292
ATOM   1845  HD2 PHE   238      -8.133  14.083  29.339
ATOM   1846  CE1 PHE   238      -7.284  14.705  25.658
ATOM   1847  HE1 PHE   238      -7.041  14.884  24.610
ATOM   1848  CE2 PHE   238      -8.372  13.412  27.327
ATOM   1849  HE2 PHE   238      -8.995  12.563  27.610
ATOM   1850  CZ  PHE   238      -8.069  13.632  26.005
ATOM   1851  HZ  PHE   238      -8.449  12.959  25.236
ATOM   1852  C   PHE   238      -4.669  16.628  30.474
ATOM   1853  O   PHE   238      -4.044  17.666  30.275
ATOM   1854  N   GLY   239      -4.934  16.190  31.708
ATOM   1855  HN  GLY   239      -5.453  15.316  31.875
ATOM   1856  CA  GLY   239      -4.462  16.997  32.776
ATOM   1857  HA1 GLY   239      -3.596  17.513  32.363
ATOM   1858  HA2 GLY   239      -4.219  16.286  33.566
ATOM   1859  C   GLY   239      -5.595  17.884  33.094
ATOM   1860  O   GLY   239      -5.465  18.843  33.854
ATOM   1861  N   VAL   240      -6.746  17.579  32.470
ATOM   1862  HN  VAL   240      -6.773  16.823  31.771
ATOM   1863  CA  VAL   240      -7.924  18.308  32.783
ATOM   1864  HA  VAL   240      -7.811  19.364  32.539
ATOM   1865  CB  VAL   240      -9.144  17.732  32.124
ATOM   1866  HB  VAL   240      -9.271  16.701  32.454
ATOM   1867  CG1 VAL   240     -10.370  18.567  32.528
ATOM   1868  HG1 VAL   240     -11.262  18.156  32.054
ATOM   1869  HG1 VAL   240     -10.489  18.539  33.611
ATOM   1870  HG1 VAL   240     -10.230  19.599  32.205
ATOM   1871  CG2 VAL   240      -8.898  17.656  30.608
ATOM   1872  HG2 VAL   240      -9.778  17.239  30.117
ATOM   1873  HG2 VAL   240      -8.706  18.656  30.219
ATOM   1874  HG2 VAL   240      -8.036  17.018  30.411
ATOM   1875  C   VAL   240      -8.065  18.086  34.239
ATOM   1876  O   VAL   240      -8.236  19.017  35.024
ATOM   1877  N   GLU   241      -7.969  16.804  34.626
ATOM   1878  HN  GLU   241      -7.844  16.064  33.922
ATOM   1879  CA  GLU   241      -8.041  16.465  36.006
ATOM   1880  HA  GLU   241      -8.906  16.947  36.461
ATOM   1881  CB  GLU   241      -8.182  14.954  36.261
ATOM   1882  HB1 GLU   241      -8.092  14.679  37.312
ATOM   1883  HB2 GLU   241      -7.433  14.353  35.746
ATOM   1884  CG  GLU   241      -9.530  14.381  35.813
ATOM   1885  HG1 GLU   241      -9.578  14.441  34.726
ATOM   1886  HG2 GLU   241     -10.319  14.978  36.270
ATOM   1887  CD  GLU   241      -9.606  12.933  36.280
ATOM   1888  OE1 GLU   241      -8.880  12.587  37.251
ATOM   1889  OE2 GLU   241     -10.394  12.156  35.679
ATOM   1891  C   GLU   241      -6.800  16.924  36.706
ATOM   1892  O   GLU   241      -6.877  17.477  37.800
ATOM   1893  N   THR   242      -5.612  16.729  36.094
ATOM   1894  HN  THR   242      -5.557  16.390  35.123
ATOM   1895  CA  THR   242      -4.428  17.015  36.856
ATOM   1896  HA  THR   242      -4.411  16.457  37.792
ATOM   1897  CB  THR   242      -3.146  16.638  36.166
ATOM   1898  HB  THR   242      -2.324  16.779  36.867
ATOM   1899  OG1 THR   242      -2.916  17.463  35.035
ATOM   1900  HG1 THR   242      -2.474  18.344  35.336
ATOM   1901  CG2 THR   242      -3.242  15.165  35.735
ATOM   1902  HG2 THR   242      -2.321  14.872  35.231
ATOM   1903  HG2 THR   242      -3.390  14.537  36.614
ATOM   1904  HG2 THR   242      -4.084  15.039  35.053
ATOM   1905  C   THR   242      -4.336  18.468  37.201
ATOM   1906  O   THR   242      -4.236  18.825  38.373
ATOM   1907  N   LEU   243      -4.389  19.351  36.190
ATOM   1908  HN  LEU   243      -4.562  19.024  35.228
```

```
ATOM   1909  CA  LEU   243      -4.205  20.747  36.450
ATOM   1910  HA  LEU   243      -3.282  20.883  37.014
ATOM   1911  CB  LEU   243      -4.096  21.566  35.146
ATOM   1912  HB1 LEU   243      -5.066  21.538  34.648
ATOM   1913  HB2 LEU   243      -3.327  21.109  34.524
ATOM   1914  CG  LEU   243      -3.717  23.051  35.327
ATOM   1915  HG  LEU   243      -3.512  23.550  34.380
ATOM   1916  CD2 LEU   243      -2.360  23.187  36.035
ATOM   1917  HD2 LEU   243      -2.115  24.243  36.151
ATOM   1918  HD2 LEU   243      -2.413  22.717  37.017
ATOM   1919  HD2 LEU   243      -1.589  22.699  35.440
ATOM   1920  CD1 LEU   243      -4.827  23.865  36.006
ATOM   1921  HD1 LEU   243      -4.506  24.902  36.108
ATOM   1922  HD1 LEU   243      -5.732  23.823  35.400
ATOM   1923  HD1 LEU   243      -5.031  23.450  36.993
ATOM   1924  C   LEU   243      -5.365  21.249  37.239
ATOM   1925  O   LEU   243      -5.197  21.944  38.240
ATOM   1926  N   GLY   244      -6.586  20.880  36.815
ATOM   1927  HN  GLY   244      -6.680  20.224  36.026
ATOM   1928  CA  GLY   244      -7.756  21.399  37.456
ATOM   1929  HA1 GLY   244      -8.652  21.054  36.941
ATOM   1930  HA2 GLY   244      -7.741  22.489  37.442
ATOM   1931  C   GLY   244      -7.812  20.938  38.877
ATOM   1932  O   GLY   244      -8.095  21.721  39.781
ATOM   1933  N   GLU   245      -7.545  19.641  39.112
ATOM   1934  HN  GLU   245      -7.240  19.033  38.338
ATOM   1935  CA  GLU   245      -7.681  19.101  40.431
ATOM   1936  HA  GLU   245      -8.678  19.294  40.829
ATOM   1937  CB  GLU   245      -7.485  17.575  40.478
ATOM   1938  HB1 GLU   245      -6.471  17.259  40.235
ATOM   1939  HB2 GLU   245      -8.126  17.033  39.782
ATOM   1940  CG  GLU   245      -7.777  16.963  41.850
ATOM   1941  HG1 GLU   245      -7.269  17.564  42.604
ATOM   1942  HG2 GLU   245      -7.400  15.940  41.852
ATOM   1943  CD  GLU   245      -9.285  16.984  42.067
ATOM   1944  OE1 GLU   245     -10.030  16.900  41.054
ATOM   1945  OE2 GLU   245      -9.712  17.085  43.248
ATOM   1947  C   GLU   245      -6.683  19.712  41.364
ATOM   1948  O   GLU   245      -7.024  20.092  42.483
ATOM   1949  N   SER   246      -5.418  19.833  40.926
ATOM   1950  HN  SER   246      -5.179  19.574  39.958
ATOM   1951  CA  SER   246      -4.403  20.323  41.812
ATOM   1952  HA  SER   246      -4.378  19.722  42.720
ATOM   1953  CB  SER   246      -2.999  20.278  41.186
ATOM   1954  HB1 SER   246      -2.973  20.888  40.283
ATOM   1955  HB2 SER   246      -2.739  19.251  40.926
ATOM   1956  OG  SER   246      -2.040  20.776  42.105
ATOM   1957  HG  SER   246      -1.351  21.354  41.603
ATOM   1958  C   SER   246      -4.688  21.744  42.180
ATOM   1959  O   SER   246      -4.642  22.107  43.356
ATOM   1960  N   VAL   247      -5.011  22.586  41.182
ATOM   1961  HN  VAL   247      -5.104  22.234  40.218
ATOM   1962  CA  VAL   247      -5.227  23.973  41.462
ATOM   1963  HA  VAL   247      -4.338  24.374  41.948
ATOM   1964  CB  VAL   247      -5.493  24.793  40.237
ATOM   1965  HB  VAL   247      -6.380  24.396  39.742
ATOM   1966  CG1 VAL   247      -5.725  26.250  40.668
ATOM   1967  HG1 VAL   247      -5.921  26.863  39.788
ATOM   1968  HG1 VAL   247      -6.581  26.299  41.341
ATOM   1969  HG1 VAL   247      -4.839  26.624  41.180
ATOM   1970  CG2 VAL   247      -4.314  24.619  39.264
ATOM   1971  HG2 VAL   247      -4.493  25.210  38.366
ATOM   1972  HG2 VAL   247      -3.395  24.956  39.743
ATOM   1973  HG2 VAL   247      -4.218  23.567  38.993
ATOM   1974  C   VAL   247      -6.409  24.102  42.364
ATOM   1975  O   VAL   247      -6.402  24.888  43.310
ATOM   1976  N   ALA   248      -7.453  23.295  42.119
ATOM   1977  HN  ALA   248      -7.392  22.581  41.379
```

ATOM	1978	CA	ALA	248	-8.656	23.432	42.892
ATOM	1979	HA	ALA	248	-9.059	24.434	42.743
ATOM	1980	CB	ALA	248	-9.729	22.403	42.504
ATOM	1981	HB1	ALA	248	-10.616	22.552	43.120
ATOM	1982	HB2	ALA	248	-9.991	22.528	41.454
ATOM	1983	HB3	ALA	248	-9.342	21.396	42.664
ATOM	1984	C	ALA	248	-8.330	23.220	44.333
ATOM	1985	O	ALA	248	-8.797	23.964	45.194
ATOM	1986	N	GLN	249	-7.501	22.208	44.644
ATOM	1987	HN	GLN	249	-7.065	21.636	43.907
ATOM	1988	CA	GLN	249	-7.241	21.946	46.027
ATOM	1989	HA	GLN	249	-8.175	21.712	46.538
ATOM	1990	CB	GLN	249	-6.260	20.780	46.238
ATOM	1991	HB1	GLN	249	-6.012	20.727	47.298
ATOM	1992	HB2	GLN	249	-5.366	20.971	45.645
ATOM	1993	CG	GLN	249	-6.814	19.416	45.821
ATOM	1994	HG1	GLN	249	-5.981	18.715	45.780
ATOM	1995	HG2	GLN	249	-7.278	19.530	44.841
ATOM	1996	CD	GLN	249	-7.837	18.989	46.862
ATOM	1997	OE1	GLN	249	-8.081	19.697	47.839
ATOM	1998	NE2	GLN	249	-8.454	17.796	46.653
ATOM	1999	HE2	GLN	249	-8.221	17.234	45.822
ATOM	2000	HE2	GLN	249	-9.155	17.453	47.326
ATOM	2001	C	GLN	249	-6.621	23.151	46.659
ATOM	2002	O	GLN	249	-7.124	23.660	47.660
ATOM	2003	N	LEU	250	-5.510	23.653	46.084
ATOM	2004	HN	LEU	250	-5.155	23.254	45.203
ATOM	2005	CA	LEU	250	-4.826	24.747	46.710
ATOM	2006	HA	LEU	250	-4.611	24.549	47.760
ATOM	2007	CB	LEU	250	-3.487	25.076	46.023
ATOM	2008	HB1	LEU	250	-3.058	25.950	46.511
ATOM	2009	HB2	LEU	250	-3.685	25.281	44.971
ATOM	2010	CG	LEU	250	-2.444	23.947	46.088
ATOM	2011	HG	LEU	250	-2.811	23.044	45.600
ATOM	2012	CD2	LEU	250	-2.222	23.471	47.531
ATOM	2013	HD2	LEU	250	-1.479	22.674	47.540
ATOM	2014	HD2	LEU	250	-1.868	24.304	48.138
ATOM	2015	HD2	LEU	250	-3.161	23.097	47.939
ATOM	2016	CD1	LEU	250	-1.139	24.359	45.390
ATOM	2017	HD1	LEU	250	-0.420	23.542	45.452
ATOM	2018	HD1	LEU	250	-1.341	24.585	44.344
ATOM	2019	HD1	LEU	250	-0.727	25.242	45.880
ATOM	2020	C	LEU	250	-5.629	26.012	46.665
ATOM	2021	O	LEU	250	-5.949	26.596	47.699
ATOM	2022	N	GLN	251	-5.992	26.443	45.444
ATOM	2023	HN	GLN	251	-5.814	25.836	44.631
ATOM	2024	CA	GLN	251	-6.619	27.716	45.234
ATOM	2025	HA	GLN	251	-6.095	28.543	45.713
ATOM	2026	CB	GLN	251	-6.641	28.131	43.752
ATOM	2027	HB1	GLN	251	-7.358	28.923	43.536
ATOM	2028	HB2	GLN	251	-6.903	27.314	43.079
ATOM	2029	CG	GLN	251	-5.292	28.656	43.248
ATOM	2030	HG1	GLN	251	-5.026	29.552	43.809
ATOM	2031	HG2	GLN	251	-5.376	28.895	42.188
ATOM	2032	CD	GLN	251	-4.232	27.583	43.455
ATOM	2033	OE1	GLN	251	-4.397	26.429	43.064
ATOM	2034	NE2	GLN	251	-3.099	27.976	44.099
ATOM	2035	HE2	GLN	251	-2.996	28.952	44.412
ATOM	2036	HE2	GLN	251	-2.344	27.296	44.274
ATOM	2037	C	GLN	251	-8.015	27.786	45.754
ATOM	2038	O	GLN	251	-8.381	28.778	46.383
ATOM	2039	N	ALA	252	-8.829	26.738	45.522
ATOM	2040	HN	ALA	252	-8.463	25.879	45.087
ATOM	2041	CA	ALA	252	-10.212	26.835	45.888
ATOM	2042	HA	ALA	252	-10.659	27.662	45.335
ATOM	2043	CB	ALA	252	-11.003	25.551	45.588
ATOM	2044	HB1	ALA	252	-12.042	25.686	45.887
ATOM	2045	HB2	ALA	252	-10.957	25.336	44.520

```
ATOM   2046  HB3 ALA   252     -10.570  24.719  46.144
ATOM   2047  C   ALA   252     -10.296  27.082  47.350
ATOM   2048  O   ALA   252     -10.959  28.015  47.800
ATOM   2049  N   TRP   253      -9.598  26.254  48.137
ATOM   2050  HN  TRP   253      -9.055  25.481  47.728
ATOM   2051  CA  TRP   253      -9.614  26.455  49.548
ATOM   2052  HA  TRP   253      -8.852  25.813  49.992
ATOM   2053  CB  TRP   253      -9.299  27.899  49.982
ATOM   2054  HB1 TRP   253     -10.049  28.560  49.546
ATOM   2055  HB2 TRP   253      -8.304  28.158  49.620
ATOM   2056  CG  TRP   253      -9.315  28.104  51.479
ATOM   2057  CD2 TRP   253     -10.480  28.518  52.218
ATOM   2058  CD1 TRP   253      -8.316  27.961  52.389
ATOM   2059  HD1 TRP   253      -7.297  27.656  52.152
ATOM   2060  NE1 TRP   253      -8.777  28.255  53.650
ATOM   2061  HE1 TRP   253      -8.220  28.222  54.516
ATOM   2062  CE2 TRP   253     -10.108  28.600  53.561
ATOM   2063  CE3 TRP   253     -11.754  28.804  51.810
ATOM   2064  HE3 TRP   253     -12.044  28.740  50.761
ATOM   2065  CZ2 TRP   253     -11.007  28.970  54.518
ATOM   2066  HZ2 TRP   253     -10.720  29.035  55.568
ATOM   2067  CZ3 TRP   253     -12.655  29.178  52.782
ATOM   2068  HZ3 TRP   253     -13.679  29.415  52.495
ATOM   2069  CH2 TRP   253     -12.292  29.260  54.109
ATOM   2070  HH2 TRP   253     -13.034  29.559  54.849
ATOM   2071  C   TRP   253     -10.965  26.093  50.053
ATOM   2072  O   TRP   253     -11.957  26.168  49.329
ATOM   2073  N   TRP   254     -11.027  25.676  51.330
ATOM   2074  HN  TRP   254     -10.153  25.591  51.869
ATOM   2075  CA  TRP   254     -12.265  25.345  51.964
ATOM   2076  HA  TRP   254     -12.709  26.302  52.238
ATOM   2077  CB  TRP   254     -13.222  24.508  51.098
ATOM   2078  HB1 TRP   254     -12.845  23.513  50.862
ATOM   2079  HB2 TRP   254     -13.447  24.958  50.131
ATOM   2080  CG  TRP   254     -14.568  24.270  51.736
ATOM   2081  CD2 TRP   254     -15.672  25.180  51.614
ATOM   2082  CD1 TRP   254     -15.005  23.233  52.508
ATOM   2083  HD1 TRP   254     -14.405  22.369  52.792
ATOM   2084  NE1 TRP   254     -16.315  23.440  52.874
ATOM   2085  HE1 TRP   254     -16.884  22.809  53.455
ATOM   2086  CE2 TRP   254     -16.736  24.636  52.330
ATOM   2087  CE3 TRP   254     -15.785  26.373  50.959
ATOM   2088  HE3 TRP   254     -14.950  26.796  50.401
ATOM   2089  CZ2 TRP   254     -17.938  25.280  52.402
ATOM   2090  HZ2 TRP   254     -18.773  24.859  52.962
ATOM   2091  CZ3 TRP   254     -16.998  27.020  51.033
ATOM   2092  HZ3 TRP   254     -17.127  27.975  50.523
ATOM   2093  CH2 TRP   254     -18.055  26.483  51.741
ATOM   2094  HH2 TRP   254     -19.001  27.022  51.777
ATOM   2095  C   TRP   254     -11.892  24.510  53.135
ATOM   2096  O   TRP   254     -10.746  24.081  53.258
ATOM   2097  N   TYR   255     -12.848  24.266  54.047
ATOM   2098  HN  TYR   255     -13.793  24.665  53.954
ATOM   2099  CA  TYR   255     -12.500  23.430  55.151
ATOM   2100  HA  TYR   255     -11.625  23.890  55.611
ATOM   2101  CB  TYR   255     -13.646  23.262  56.162
ATOM   2102  HB1 TYR   255     -14.489  22.816  55.633
ATOM   2103  HB2 TYR   255     -13.897  24.251  56.544
ATOM   2104  CG  TYR   255     -13.159  22.369  57.251
ATOM   2105  CD1 TYR   255     -12.398  22.875  58.280
ATOM   2106  HD1 TYR   255     -12.151  23.937  58.297
ATOM   2107  CD2 TYR   255     -13.464  21.027  57.247
ATOM   2108  HD2 TYR   255     -14.067  20.614  56.439
ATOM   2109  CE1 TYR   255     -11.946  22.054  59.289
ATOM   2110  HE1 TYR   255     -11.344  22.465  60.099
ATOM   2111  CE2 TYR   255     -13.016  20.203  58.250
ATOM   2112  HE2 TYR   255     -13.264  19.142  58.234
ATOM   2113  CZ  TYR   255     -12.256  20.715  59.273
```

	ATOM	2114	OH	TYR	255	-11.794	19.871	60.306
	ATOM	2115	HH	TYR	255	-12.089	20.249	61.217
	ATOM	2116	C	TYR	255	-12.207	22.088	54.573
	ATOM	2117	O	TYR	255	-11.103	21.563	54.704
5	ATOM	2118	N	LYS	256	-13.211	21.508	53.889
	ATOM	2119	HN	LYS	256	-14.108	22.005	53.789
	ATOM	2120	CA	LYS	256	-13.057	20.216	53.301
	ATOM	2121	HA	LYS	256	-12.623	19.534	54.032
	ATOM	2122	CB	LYS	256	-14.390	19.614	52.820
10	ATOM	2123	HB1	LYS	256	-15.152	19.558	53.597
	ATOM	2124	HB2	LYS	256	-14.301	18.596	52.441
	ATOM	2125	CG	LYS	256	-15.045	20.400	51.683
	ATOM	2126	HG1	LYS	256	-14.357	20.653	50.876
	ATOM	2127	HG2	LYS	256	-15.472	21.351	52.002
15	ATOM	2128	CD	LYS	256	-16.195	19.651	51.008
	ATOM	2129	HD1	LYS	256	-16.765	20.263	50.308
	ATOM	2130	HD2	LYS	256	-16.934	19.261	51.708
	ATOM	2131	CE	LYS	256	-15.742	18.436	50.194
	ATOM	2132	HE1	LYS	256	-15.231	17.724	50.841
20	ATOM	2133	HE2	LYS	256	-15.060	18.751	49.404
	ATOM	2134	NZ	LYS	256	-16.914	17.774	49.580
	ATOM	2135	HZ1	LYS	256	-16.602	16.958	49.034
	ATOM	2136	HZ2	LYS	256	-17.561	17.464	50.320
	ATOM	2137	HZ3	LYS	256	-17.398	18.437	48.958
25	ATOM	2138	C	LYS	256	-12.155	20.315	52.114
	ATOM	2139	O	LYS	256	-11.245	19.503	51.957
	ATOM	2140	N	ALA	257	-12.376	21.329	51.252
	ATOM	2141	HN	ALA	257	-13.096	22.037	51.456
	ATOM	2142	CA	ALA	257	-11.599	21.410	50.048
30	ATOM	2143	HA	ALA	257	-11.784	20.515	49.454
	ATOM	2144	CB	ALA	257	-11.938	22.647	49.200
	ATOM	2145	HB1	ALA	257	-11.318	22.654	48.303
	ATOM	2146	HB2	ALA	257	-12.989	22.617	48.914
	ATOM	2147	HB3	ALA	257	-11.746	23.550	49.780
35	ATOM	2148	C	ALA	257	-10.158	21.498	50.418
	ATOM	2149	O	ALA	257	-9.392	20.567	50.170
	ATOM	2150	N	ASP	258	-9.744	22.615	51.041
	ATOM	2151	HN	ASP	258	-10.388	23.400	51.215
	ATOM	2152	CA	ASP	258	-8.377	22.671	51.454
40	ATOM	2153	HA	ASP	258	-8.195	21.850	52.147
	ATOM	2154	CB	ASP	258	-7.380	22.568	50.287
	ATOM	2155	HB1	ASP	258	-7.433	23.495	49.715
	ATOM	2156	HB2	ASP	258	-7.666	21.715	49.672
	ATOM	2157	CG	ASP	258	-5.989	22.372	50.871
45	ATOM	2158	OD1	ASP	258	-5.879	22.319	52.126
	ATOM	2159	OD2	ASP	258	-5.020	22.265	50.073
	ATOM	2160	C	ASP	258	-8.144	23.982	52.120
	ATOM	2161	O	ASP	258	-8.499	25.035	51.601
	ATOM	2162	N	PRO	259	-7.550	23.942	53.269
50	ATOM	2163	CA	PRO	259	-7.232	25.190	53.902
	ATOM	2164	HA	PRO	259	-7.984	25.946	53.675
	ATOM	2165	CD	PRO	259	-7.971	22.940	54.235
	ATOM	2166	HD1	PRO	259	-7.192	22.177	54.227
	ATOM	2167	HD2	PRO	259	-8.932	22.570	53.878
55	ATOM	2168	CB	PRO	259	-7.168	24.904	55.399
	ATOM	2169	HB1	PRO	259	-7.531	25.757	55.974
	ATOM	2170	HB2	PRO	259	-6.145	24.697	55.712
	ATOM	2171	CG	PRO	259	-8.074	23.675	55.580
	ATOM	2172	HG1	PRO	259	-9.100	23.976	55.794
60	ATOM	2173	HG2	PRO	259	-7.726	23.053	56.405
	ATOM	2174	C	PRO	259	-5.908	25.542	53.327
	ATOM	2175	O	PRO	259	-5.446	24.799	52.464
	ATOM	2176	N	ASN	260	-5.281	26.651	53.759
	ATOM	2177	HN	ASN	260	-5.719	27.281	54.445
65	ATOM	2178	CA	ASN	260	-3.980	26.920	53.225
	ATOM	2179	HA	ASN	260	-4.106	27.027	52.148
	ATOM	2180	CB	ASN	260	-3.353	28.235	53.743
	ATOM	2181	HB1	ASN	260	-3.969	29.085	53.449

	ATOM	2182	HB2	ASN	260	-2.354	28.363	53.326
	ATOM	2183	CG	ASN	260	-3.251	28.203	55.262
	ATOM	2184	OD1	ASN	260	-4.209	27.862	55.954
	ATOM	2185	ND2	ASN	260	-2.054	28.565	55.798
5	ATOM	2186	HD2	ASN	260	-1.278	28.844	55.182
	ATOM	2187	HD2	ASN	260	-1.925	28.559	56.820
	ATOM	2188	C	ASN	260	-3.126	25.747	53.586
	ATOM	2189	O	ASN	260	-2.726	25.572	54.737
	ATOM	2190	N	ASP	261	-2.842	24.884	52.593
10	ATOM	2191	HN	ASP	261	-3.151	25.083	51.630
	ATOM	2192	CA	ASP	261	-2.111	23.690	52.879
	ATOM	2193	HA	ASP	261	-1.559	23.824	53.809
	ATOM	2194	CB	ASP	261	-2.994	22.434	53.010
	ATOM	2195	HB1	ASP	261	-2.359	21.549	52.988
15	ATOM	2196	HB2	ASP	261	-3.699	22.407	52.179
	ATOM	2197	CG	ASP	261	-3.753	22.496	54.330
	ATOM	2198	OD1	ASP	261	-3.245	23.148	55.280
	ATOM	2199	OD2	ASP	261	-4.850	21.882	54.408
	ATOM	2200	C	ASP	261	-1.161	23.420	51.762
20	ATOM	2201	O	ASP	261	-1.063	24.177	50.797
	ATOM	2202	N	PHE	262	-0.424	22.304	51.918
	ATOM	2203	HN	PHE	262	-0.588	21.752	52.771
	ATOM	2204	CA	PHE	262	0.566	21.814	51.008
	ATOM	2205	HA	PHE	262	0.703	22.623	50.290
25	ATOM	2206	CB	PHE	262	1.823	21.407	51.796
	ATOM	2207	HB1	PHE	262	1.645	20.525	52.411
	ATOM	2208	HB2	PHE	262	2.157	22.202	52.462
	ATOM	2209	CG	PHE	262	2.957	21.088	50.893
	ATOM	2210	CD1	PHE	262	3.827	22.077	50.497
30	ATOM	2211	HD1	PHE	262	3.675	23.100	50.844
	ATOM	2212	CD2	PHE	262	3.157	19.800	50.461
	ATOM	2213	HD2	PHE	262	2.477	19.009	50.776
	ATOM	2214	CE1	PHE	262	4.885	21.789	49.670
	ATOM	2215	HE1	PHE	262	5.569	22.579	49.359
35	ATOM	2216	CE2	PHE	262	4.212	19.509	49.634
	ATOM	2217	HE2	PHE	262	4.363	18.485	49.290
	ATOM	2218	CZ	PHE	262	5.078	20.499	49.236
	ATOM	2219	HZ	PHE	262	5.915	20.262	48.579
	ATOM	2220	C	PHE	262	-0.039	20.576	50.420
40	ATOM	2221	O	PHE	262	-0.720	19.836	51.128
	ATOM	2222	N	THR	263	0.152	20.313	49.109
	ATOM	2223	HN	THR	263	0.725	20.929	48.514
	ATOM	2224	CA	THR	263	-0.479	19.134	48.583
	ATOM	2225	HA	THR	263	-0.713	18.443	49.392
45	ATOM	2226	CB	THR	263	-1.753	19.421	47.846
	ATOM	2227	HB	THR	263	-1.533	20.090	47.014
	ATOM	2228	OG1	THR	263	-2.686	20.055	48.709
	ATOM	2229	HG1	THR	263	-2.364	21.009	48.923
	ATOM	2230	CG2	THR	263	-2.331	18.096	47.324
50	ATOM	2231	HG2	THR	263	-3.259	18.290	46.786
	ATOM	2232	HG2	THR	263	-1.614	17.625	46.652
	ATOM	2233	HG2	THR	263	-2.531	17.430	48.164
	ATOM	2234	C	THR	263	0.435	18.451	47.613
	ATOM	2235	O	THR	263	1.217	19.096	46.917
55	ATOM	2236	N	TYR	264	0.361	17.101	47.562
	ATOM	2237	HN	TYR	264	-0.251	16.601	48.221
	ATOM	2238	CA	TYR	264	1.128	16.359	46.603
	ATOM	2239	HA	TYR	264	1.472	17.073	45.855
	ATOM	2240	CB	TYR	264	2.376	15.650	47.166
60	ATOM	2241	HB1	TYR	264	2.989	16.340	47.746
	ATOM	2242	HB2	TYR	264	2.994	15.248	46.363
	ATOM	2243	CG	TYR	264	1.993	14.520	48.058
	ATOM	2244	CD1	TYR	264	1.649	14.735	49.373
	ATOM	2245	HD1	TYR	264	1.647	15.748	49.773
65	ATOM	2246	CD2	TYR	264	1.998	13.233	47.571
	ATOM	2247	HD2	TYR	264	2.276	13.052	46.532
	ATOM	2248	CE1	TYR	264	1.308	13.678	50.184
	ATOM	2249	HE1	TYR	264	1.034	13.856	51.224

ATOM	2250	CE2	TYR	264	1.658	12.173	48.377
ATOM	2251	HE2	TYR	264	1.664	11.159	47.977
ATOM	2252	CZ	TYR	264	1.311	12.395	49.686
ATOM	2253	OH	TYR	264	0.963	11.309	50.515
ATOM	2254	HH	TYR	264	0.276	11.618	51.217
ATOM	2255	C	TYR	264	0.210	15.332	46.020
ATOM	2256	O	TYR	264	-0.838	15.027	46.587
ATOM	2257	N	GLU	265	0.584	14.773	44.852
ATOM	2258	HN	GLU	265	1.508	14.994	44.453
ATOM	2259	CA	GLU	265	-0.291	13.872	44.161
ATOM	2260	HA	GLU	265	-1.208	13.769	44.741
ATOM	2261	CB	GLU	265	-0.621	14.429	42.767
ATOM	2262	HB1	GLU	265	0.233	14.234	42.120
ATOM	2263	HB2	GLU	265	-0.800	15.500	42.871
ATOM	2264	CG	GLU	265	-1.844	13.843	42.070
ATOM	2265	HG1	GLU	265	-2.611	13.771	42.841
ATOM	2266	HG2	GLU	265	-1.526	12.872	41.691
ATOM	2267	CD	GLU	265	-2.196	14.831	40.966
ATOM	2268	OE1	GLU	265	-1.626	15.954	40.985
ATOM	2269	OE2	GLU	265	-3.036	14.489	40.095
ATOM	2271	C	GLU	265	0.397	12.546	44.028
ATOM	2272	O	GLU	265	1.598	12.434	44.271
ATOM	2273	N	ARG	266	-0.365	11.493	43.665
ATOM	2274	HN	ARG	266	-1.369	11.637	43.486
ATOM	2275	CA	ARG	266	0.189	10.175	43.523
ATOM	2276	HA	ARG	266	0.892	10.012	44.340
ATOM	2277	CB	ARG	266	-0.855	9.046	43.540
ATOM	2278	HB1	ARG	266	-0.451	8.069	43.275
ATOM	2279	HB2	ARG	266	-1.682	9.202	42.848
ATOM	2280	CG	ARG	266	-1.517	8.839	44.901
ATOM	2281	HG1	ARG	266	-2.192	9.648	45.183
ATOM	2282	HG2	ARG	266	-0.805	8.762	45.723
ATOM	2283	CD	ARG	266	-2.361	7.566	44.981
ATOM	2284	HD1	ARG	266	-1.734	6.737	44.651
ATOM	2285	HD2	ARG	266	-3.220	7.702	44.324
ATOM	2286	NE	ARG	266	-2.783	7.398	46.400
ATOM	2287	HE	ARG	266	-2.869	8.221	47.013
ATOM	2288	CZ	ARG	266	-3.055	6.152	46.886
ATOM	2289	NH1	ARG	266	-2.958	5.065	46.067
ATOM	2290	HH1	ARG	266	-3.163	4.124	46.433
ATOM	2291	HH1	ARG	266	-2.679	5.184	45.083
ATOM	2292	NH2	ARG	266	-3.413	5.992	48.193
ATOM	2293	HH2	ARG	266	-3.619	5.052	48.560
ATOM	2294	HH2	ARG	266	-3.478	6.812	48.813
ATOM	2295	C	ARG	266	0.881	10.104	42.208
ATOM	2296	O	ARG	266	0.463	10.727	41.235
ATOM	2297	N	ARG	267	1.979	9.329	42.154
ATOM	2298	HN	ARG	267	2.288	8.803	42.984
ATOM	2299	CA	ARG	267	2.710	9.246	40.932
ATOM	2300	HA	ARG	267	2.245	9.909	40.202
ATOM	2301	CB	ARG	267	4.190	9.606	41.128
ATOM	2302	HB1	ARG	267	4.777	9.522	40.213
ATOM	2303	HB2	ARG	267	4.693	8.969	41.857
ATOM	2304	CG	ARG	267	4.400	11.039	41.622
ATOM	2305	HG1	ARG	267	3.662	11.363	42.356
ATOM	2306	HG2	ARG	267	4.354	11.787	40.830
ATOM	2307	CD	ARG	267	5.754	11.265	42.299
ATOM	2308	HD1	ARG	267	5.861	10.534	43.100
ATOM	2309	HD2	ARG	267	5.772	12.279	42.697
ATOM	2310	NE	ARG	267	6.821	11.084	41.278
ATOM	2311	HE	ARG	267	6.571	10.906	40.294
ATOM	2312	CZ	ARG	267	8.133	11.155	41.650
ATOM	2313	NH1	ARG	267	8.459	11.363	42.958
ATOM	2314	HH1	ARG	267	9.448	11.417	43.241
ATOM	2315	HH1	ARG	267	7.716	11.466	43.664
ATOM	2316	NH2	ARG	267	9.119	11.022	40.715
ATOM	2317	HH2	ARG	267	10.108	11.076	40.998
ATOM	2318	HH2	ARG	267	8.874	10.866	39.727

```
ATOM   2319  C   ARG  267      2.670   7.832  40.447
ATOM   2320  O   ARG  267      3.493   7.010  40.846
ATOM   2321  N   LYS  268      1.696   7.504  39.573
ATOM   2322  HN  LYS  268      0.934   8.168  39.374
ATOM   2323  CA  LYS  268      1.725   6.226  38.922
ATOM   2324  HA  LYS  268      2.350   5.512  39.457
ATOM   2325  CB  LYS  268      0.324   5.630  38.681
ATOM   2326  HB1 LYS  268     -0.100   6.107  37.798
ATOM   2327  HB2 LYS  268     -0.285   5.831  39.561
ATOM   2328  CG  LYS  268      0.298   4.114  38.442
ATOM   2329  HG1 LYS  268     -0.741   3.808  38.327
ATOM   2330  HG2 LYS  268      0.752   3.628  39.305
ATOM   2331  CD  LYS  268      1.053   3.636  37.200
ATOM   2332  HD1 LYS  268      2.115   3.884  37.210
ATOM   2333  HD2 LYS  268      0.677   4.058  36.268
ATOM   2334  CE  LYS  268      1.004   2.121  36.994
ATOM   2335  HE1 LYS  268     -0.029   1.790  36.904
ATOM   2336  HE2 LYS  268      1.465   1.614  37.843
ATOM   2337  NZ  LYS  268      1.735   1.753  35.761
ATOM   2338  HZ1 LYS  268      1.697   0.732  35.630
ATOM   2339  HZ2 LYS  268      1.301   2.218  34.951
ATOM   2340  HZ3 LYS  268      2.718   2.052  35.841
ATOM   2341  C   LYS  268      2.286   6.620  37.609
ATOM   2342  O   LYS  268      1.912   6.148  36.538
ATOM   2343  N   GLU  269      3.252   7.535  37.708
ATOM   2344  HN  GLU  269      3.548   7.838  38.648
ATOM   2345  CA  GLU  269      3.888   8.108  36.585
ATOM   2346  HA  GLU  269      3.128   8.660  36.033
ATOM   2347  CB  GLU  269      5.011   9.051  37.041
ATOM   2348  HB1 GLU  269      4.624   9.960  37.503
ATOM   2349  HB2 GLU  269      5.645   9.369  36.214
ATOM   2350  CG  GLU  269      5.932   8.398  38.071
ATOM   2351  HG1 GLU  269      6.587   7.698  37.551
ATOM   2352  HG2 GLU  269      5.315   7.874  38.801
ATOM   2353  CD  GLU  269      6.747   9.491  38.748
ATOM   2354  OE1 GLU  269      6.550  10.684  38.397
ATOM   2355  OE2 GLU  269      7.582   9.140  39.624
ATOM   2357  C   GLU  269      4.445   6.994  35.785
ATOM   2358  O   GLU  269      4.595   5.872  36.266
ATOM   2359  N   SER  270      4.748   7.289  34.511
ATOM   2360  HN  SER  270      4.513   8.219  34.136
ATOM   2361  CA  SER  270      5.391   6.332  33.670
ATOM   2362  HA  SER  270      4.828   5.409  33.807
ATOM   2363  CB  SER  270      5.425   6.707  32.177
ATOM   2364  HB1 SER  270      4.414   6.802  31.783
ATOM   2365  HB2 SER  270      5.947   5.941  31.603
ATOM   2366  OG  SER  270      6.097   7.942  31.989
ATOM   2367  HG  SER  270      7.063   7.865  32.339
ATOM   2368  C   SER  270      6.788   6.252  34.170
ATOM   2369  O   SER  270      7.575   5.432  33.704
ATOM   2370  N   ALA  271      7.150   7.171  35.098
ATOM   2371  HN  ALA  271      6.456   7.880  35.376
ATOM   2372  CA  ALA  271      8.442   7.213  35.715
ATOM   2373  HA  ALA  271      9.145   7.337  34.891
ATOM   2374  CB  ALA  271      8.599   8.254  36.825
ATOM   2375  HB1 ALA  271      9.610   8.207  37.228
ATOM   2376  HB2 ALA  271      8.416   9.249  36.419
ATOM   2377  HB3 ALA  271      7.882   8.049  37.620
ATOM   2378  C   ALA  271      8.575   5.925  36.412
ATOM   2379  O   ALA  271      9.693   5.491  36.685
ATOM   2380  N   ALA  272      7.405   5.344  36.761
ATOM   2381  HN  ALA  272      6.531   5.865  36.603
ATOM   2382  CA  ALA  272      7.326   4.044  37.337
ATOM   2383  HA  ALA  272      7.642   4.176  38.372
ATOM   2384  CB  ALA  272      5.925   3.420  37.214
ATOM   2385  HB1 ALA  272      5.927   2.430  37.670
ATOM   2386  HB2 ALA  272      5.199   4.053  37.723
ATOM   2387  HB3 ALA  272      5.656   3.333  36.161
```

ATOM	2388	C	ALA	272	8.258	3.213	36.532
ATOM	2389	O	ALA	272	9.072	2.473	37.074
ATOM	2390	N	TYR	273	8.199	3.402	35.202
ATOM	2391	HN	TYR	273	7.478	4.034	34.825
ATOM	2392	CA	TYR	273	9.094	2.763	34.289
ATOM	2393	HA	TYR	273	9.209	1.748	34.668
ATOM	2394	CB	TYR	273	8.643	2.876	32.821
ATOM	2395	HB1	TYR	273	9.331	2.333	32.173
ATOM	2396	HB2	TYR	273	8.623	3.922	32.513
ATOM	2397	CG	TYR	273	7.278	2.304	32.656
ATOM	2398	CD1	TYR	273	6.173	3.097	32.864
ATOM	2399	HD1	TYR	273	6.306	4.140	33.152
ATOM	2400	CD2	TYR	273	7.095	0.988	32.298
ATOM	2401	HD2	TYR	273	7.961	0.346	32.134
ATOM	2402	CE1	TYR	273	4.904	2.592	32.713
ATOM	2403	HE1	TYR	273	4.038	3.232	32.878
ATOM	2404	CE2	TYR	273	5.827	0.476	32.144
ATOM	2405	HE2	TYR	273	5.692	-0.565	31.856
ATOM	2406	CZ	TYR	273	4.730	1.278	32.353
ATOM	2407	OH	TYR	273	3.429	0.754	32.197
ATOM	2408	HH	TYR	273	2.736	1.500	32.352
ATOM	2409	C	TYR	273	10.354	3.569	34.349
ATOM	2410	O	TYR	273	10.407	4.679	33.822
ATOM	2411	N	ILE	274	11.407	3.044	35.002
ATOM	2412	HN	ILE	274	11.340	2.124	35.459
ATOM	2413	CA	ILE	274	12.624	3.798	35.044
ATOM	2414	HA	ILE	274	12.412	4.791	34.648
ATOM	2415	CB	ILE	274	13.248	3.924	36.406
ATOM	2416	HB	ILE	274	13.303	2.917	36.820
ATOM	2417	CG2	ILE	274	14.642	4.542	36.198
ATOM	2418	HG2	ILE	274	15.139	4.654	37.162
ATOM	2419	HG2	ILE	274	15.237	3.890	35.558
ATOM	2420	HG2	ILE	274	14.541	5.519	35.726
ATOM	2421	CG1	ILE	274	12.374	4.755	37.358
ATOM	2422	HG1	ILE	274	12.729	4.732	38.388
ATOM	2423	HG1	ILE	274	11.340	4.412	37.392
ATOM	2424	CD1	ILE	274	12.311	6.232	36.971
ATOM	2425	HD1	ILE	274	11.679	6.767	37.680
ATOM	2426	HD1	ILE	274	13.315	6.656	36.989
ATOM	2427	HD1	ILE	274	11.894	6.328	35.969
ATOM	2428	C	ILE	274	13.625	3.087	34.206
ATOM	2429	O	ILE	274	13.749	1.865	34.243
ATOM	2430	N	PRO	275	14.308	3.853	33.410
ATOM	2431	CA	PRO	275	15.358	3.271	32.630
ATOM	2432	HA	PRO	275	15.019	2.296	32.281
ATOM	2433	CD	PRO	275	13.627	4.919	32.691
ATOM	2434	HD1	PRO	275	13.856	5.834	33.236
ATOM	2435	HD2	PRO	275	12.569	4.660	32.716
ATOM	2436	CB	PRO	275	15.576	4.204	31.441
ATOM	2437	HB1	PRO	275	15.854	3.642	30.550
ATOM	2438	HB2	PRO	275	16.373	4.919	31.648
ATOM	2439	CG	PRO	275	14.216	4.902	31.272
ATOM	2440	HG1	PRO	275	13.678	4.265	30.570
ATOM	2441	HG2	PRO	275	14.472	5.887	30.880
ATOM	2442	C	PRO	275	16.561	3.135	33.500
ATOM	2443	O	PRO	275	16.674	3.878	34.473
ATOM	2444	N	PHE	276	17.462	2.188	33.190
ATOM	2445	HN	PHE	276	17.302	1.551	32.396
ATOM	2446	CA	PHE	276	18.649	2.082	33.981
ATOM	2447	HA	PHE	276	18.748	3.018	34.529
ATOM	2448	CB	PHE	276	18.613	0.964	35.044
ATOM	2449	HB1	PHE	276	17.772	1.094	35.726
ATOM	2450	HB2	PHE	276	19.524	0.957	35.641
ATOM	2451	CG	PHE	276	18.477	-0.377	34.412
ATOM	2452	CD1	PHE	276	17.278	-0.790	33.879
ATOM	2453	HD1	PHE	276	16.417	-0.122	33.908
ATOM	2454	CD2	PHE	276	19.548	-1.240	34.388
ATOM	2455	HD2	PHE	276	20.499	-0.933	34.823

ATOM	2456	CE1	PHE	276	17.152	-2.035	33.309
ATOM	2457	HE1	PHE	276	16.199	-2.347	32.884
ATOM	2458	CE2	PHE	276	19.428	-2.485	33.821
ATOM	2459	HE2	PHE	276	20.285	-3.158	33.801
ATOM	2460	CZ	PHE	276	18.231	-2.885	33.278
ATOM	2461	HZ	PHE	276	18.137	-3.872	32.826
ATOM	2462	C	PHE	276	19.780	1.866	33.036
ATOM	2463	O	PHE	276	19.649	2.139	31.844
ATOM	2464	N	GLY	277	20.933	1.399	33.552
ATOM	2465	HN	GLY	277	20.993	1.171	34.555
ATOM	2466	CA	GLY	277	22.078	1.219	32.707
ATOM	2467	HA1	GLY	277	22.869	0.759	33.300
ATOM	2468	HA2	GLY	277	22.389	2.198	32.342
ATOM	2469	C	GLY	277	21.685	0.333	31.573
ATOM	2470	O	GLY	277	21.690	0.754	30.417
ATOM	2471	N	GLU	278	21.332	-0.927	31.877
ATOM	2472	HN	GLU	278	21.354	-1.255	32.852
ATOM	2473	CA	GLU	278	20.924	-1.806	30.824
ATOM	2474	HA	GLU	278	21.695	-1.768	30.054
ATOM	2475	CB	GLU	278	20.707	-3.257	31.283
ATOM	2476	HB1	GLU	278	19.940	-3.358	32.051
ATOM	2477	HB2	GLU	278	21.600	-3.716	31.707
ATOM	2478	CG	GLU	278	20.271	-4.193	30.154
ATOM	2479	HG1	GLU	278	21.078	-4.233	29.422
ATOM	2480	HG2	GLU	278	19.363	-3.784	29.711
ATOM	2481	CD	GLU	278	20.013	-5.565	30.757
ATOM	2482	OE1	GLU	278	20.174	-5.708	31.998
ATOM	2483	OE2	GLU	278	19.644	-6.489	29.985
ATOM	2485	C	GLU	278	19.614	-1.308	30.315
ATOM	2486	O	GLU	278	19.391	-1.243	29.106
ATOM	2487	N	GLY	279	18.714	-0.913	31.236
ATOM	2488	HN	GLY	279	18.958	-0.916	32.237
ATOM	2489	CA	GLY	279	17.415	-0.491	30.809
ATOM	2490	HA1	GLY	279	17.593	0.375	30.172
ATOM	2491	HA2	GLY	279	16.877	-0.251	31.727
ATOM	2492	C	GLY	279	16.847	-1.659	30.077
ATOM	2493	O	GLY	279	17.294	-2.791	30.256
ATOM	2494	N	ASP	280	15.838	-1.416	29.222
ATOM	2495	HN	ASP	280	15.446	-2.191	28.668
ATOM	2496	CA	ASP	280	15.300	-0.101	29.069
ATOM	2497	HA	ASP	280	16.143	0.583	28.983
ATOM	2498	CB	ASP	280	14.374	0.016	27.846
ATOM	2499	HB1	ASP	280	13.494	-0.606	28.011
ATOM	2500	HB2	ASP	280	14.914	-0.324	26.963
ATOM	2501	CG	ASP	280	13.963	1.472	27.681
ATOM	2502	OD1	ASP	280	14.347	2.304	28.546
ATOM	2503	OD2	ASP	280	13.253	1.772	26.683
ATOM	2504	C	ASP	280	14.479	0.184	30.284
ATOM	2505	O	ASP	280	14.579	1.251	30.884
ATOM	2506	N	PHE	281	13.646	-0.795	30.682
ATOM	2507	HN	PHE	281	13.659	-1.694	30.179
ATOM	2508	CA	PHE	281	12.741	-0.630	31.782
ATOM	2509	HA	PHE	281	12.875	0.368	32.198
ATOM	2510	CB	PHE	281	11.293	-0.827	31.297
ATOM	2511	HB1	PHE	281	11.206	-1.698	30.647
ATOM	2512	HB2	PHE	281	10.941	0.036	30.734
ATOM	2513	CG	PHE	281	10.361	-1.027	32.436
ATOM	2514	CD1	PHE	281	9.885	0.033	33.169
ATOM	2515	HD1	PHE	281	10.200	1.048	32.926
ATOM	2516	CD2	PHE	281	9.949	-2.302	32.748
ATOM	2517	HD2	PHE	281	10.319	-3.145	32.165
ATOM	2518	CE1	PHE	281	9.013	-0.183	34.208
ATOM	2519	HE1	PHE	281	8.637	0.658	34.788
ATOM	2520	CE2	PHE	281	9.078	-2.525	33.785
ATOM	2521	HE2	PHE	281	8.757	-3.539	34.025
ATOM	2522	CZ	PHE	281	8.615	-1.461	34.516
ATOM	2523	HZ	PHE	281	7.928	-1.631	35.346
ATOM	2524	C	PHE	281	13.051	-1.666	32.816

	ATOM	2525	O	PHE	281	12.644	-2.819	32.681
	ATOM	2526	N	TYR	282	13.810	-1.295	33.871
	ATOM	2527	HN	TYR	282	14.179	-0.338	33.954
	ATOM	2528	CA	TYR	282	14.079	-2.287	34.870
5	ATOM	2529	HA	TYR	282	14.418	-3.216	34.411
	ATOM	2530	CB	TYR	282	15.293	-1.981	35.778
	ATOM	2531	HB1	TYR	282	16.230	-1.942	35.223
	ATOM	2532	HB2	TYR	282	15.431	-2.731	36.557
	ATOM	2533	CG	TYR	282	15.167	-0.672	36.477
10	ATOM	2534	CD1	TYR	282	15.505	0.501	35.847
	ATOM	2535	HD1	TYR	282	15.862	0.477	34.817
	ATOM	2536	CD2	TYR	282	14.742	-0.622	37.780
	ATOM	2537	HD2	TYR	282	14.488	-1.547	38.298
	ATOM	2538	CE1	TYR	282	15.397	1.706	36.502
15	ATOM	2539	HE1	TYR	282	15.660	2.631	35.988
	ATOM	2540	CE2	TYR	282	14.631	0.575	38.441
	ATOM	2541	HE2	TYR	282	14.283	0.597	39.474
	ATOM	2542	CZ	TYR	282	14.958	1.744	37.803
	ATOM	2543	OH	TYR	282	14.843	2.972	38.488
20	ATOM	2544	HH	TYR	282	15.739	3.478	38.440
	ATOM	2545	C	TYR	282	12.844	-2.583	35.672
	ATOM	2546	O	TYR	282	12.471	-3.748	35.808
	ATOM	2547	N	TYR	283	12.148	-1.559	36.218
	ATOM	2548	HN	TYR	283	12.481	-0.586	36.153
25	ATOM	2549	CA	TYR	283	10.918	-1.889	36.894
	ATOM	2550	HA	TYR	283	10.394	-2.679	36.357
	ATOM	2551	CB	TYR	283	11.029	-2.502	38.313
	ATOM	2552	HB1	TYR	283	11.706	-3.355	38.358
	ATOM	2553	HB2	TYR	283	10.076	-2.862	38.698
30	ATOM	2554	CG	TYR	283	11.533	-1.535	39.329
	ATOM	2555	CD1	TYR	283	10.709	-0.556	39.836
	ATOM	2556	HD1	TYR	283	9.678	-0.487	39.488
	ATOM	2557	CD2	TYR	283	12.828	-1.607	39.784
	ATOM	2558	HD2	TYR	283	13.494	-2.377	39.395
35	ATOM	2559	CE1	TYR	283	11.168	0.336	40.777
	ATOM	2560	HE1	TYR	283	10.505	1.108	41.166
	ATOM	2561	CE2	TYR	283	13.295	-0.719	40.725
	ATOM	2562	HE2	TYR	283	14.325	-0.788	41.076
	ATOM	2563	CZ	TYR	283	12.464	0.254	41.223
40	ATOM	2564	OH	TYR	283	12.941	1.166	42.189
	ATOM	2565	HH	TYR	283	13.805	1.609	41.846
	ATOM	2566	C	TYR	283	10.032	-0.688	36.969
	ATOM	2567	O	TYR	283	10.398	0.392	36.511
	ATOM	2568	N	HIS	284	8.817	-0.883	37.540
45	ATOM	2569	HN	HIS	284	8.615	-1.813	37.932
	ATOM	2570	CA	HIS	284	7.789	0.121	37.635
	ATOM	2571	HA	HIS	284	8.024	0.930	36.944
	ATOM	2572	ND1	HIS	284	6.216	-2.488	35.948
	ATOM	2573	HD1	HIS	284	6.497	-3.176	36.660
50	ATOM	2574	CG	HIS	284	6.112	-1.124	36.119
	ATOM	2575	NE2	HIS	284	5.564	-1.651	33.995
	ATOM	2576	HE2	HIS	284	5.274	-1.572	33.009
	ATOM	2577	CD2	HIS	284	5.715	-0.630	34.916
	ATOM	2578	HD2	HIS	284	5.539	0.425	34.707
55	ATOM	2579	CE1	HIS	284	5.876	-2.748	34.660
	ATOM	2580	HE1	HIS	284	5.861	-3.748	34.225
	ATOM	2581	CB	HIS	284	6.363	-0.420	37.419
	ATOM	2582	HB1	HIS	284	5.676	0.424	37.461
	ATOM	2583	HB2	HIS	284	6.154	-1.135	38.214
60	ATOM	2584	C	HIS	284	7.749	0.638	39.040
	ATOM	2585	O	HIS	284	8.007	-0.096	39.993
	ATOM	2586	N	ALA	285	7.424	1.937	39.207
	ATOM	2587	HN	ALA	285	7.259	2.541	38.390
	ATOM	2588	CA	ALA	285	7.310	2.469	40.534
65	ATOM	2589	HA	ALA	285	7.116	1.651	41.228
	ATOM	2590	CB	ALA	285	8.568	3.217	41.007
	ATOM	2591	HB1	ALA	285	8.410	3.592	42.018
	ATOM	2592	HB2	ALA	285	9.420	2.537	41.001

ATOM	2593	HB3	ALA	285	8.767	4.054	40.337
ATOM	2594	C	ALA	285	6.179	3.450	40.570
ATOM	2595	O	ALA	285	6.114	4.387	39.774
ATOM	2596	N	ALA	286	5.240	3.250	41.512
ATOM	2597	HN	ALA	286	5.293	2.426	42.127
ATOM	2598	CA	ALA	286	4.165	4.186	41.658
ATOM	2599	HA	ALA	286	4.386	5.003	40.971
ATOM	2600	CB	ALA	286	2.776	3.583	41.385
ATOM	2601	HB1	ALA	286	2.014	4.351	41.516
ATOM	2602	HB2	ALA	286	2.738	3.204	40.364
ATOM	2603	HB3	ALA	286	2.591	2.766	42.083
ATOM	2604	C	ALA	286	4.186	4.609	43.083
ATOM	2605	O	ALA	286	4.231	3.771	43.983
ATOM	2606	N	ILE	287	4.182	5.928	43.340
ATOM	2607	HN	ILE	287	4.190	6.628	42.584
ATOM	2608	CA	ILE	287	4.165	6.306	44.716
ATOM	2609	HA	ILE	287	4.350	5.406	45.303
ATOM	2610	CB	ILE	287	5.221	7.292	45.121
ATOM	2611	HB	ILE	287	6.199	6.912	44.827
ATOM	2612	CG2	ILE	287	4.954	8.635	44.421
ATOM	2613	HG2	ILE	287	5.718	9.355	44.712
ATOM	2614	HG2	ILE	287	4.981	8.494	43.341
ATOM	2615	HG2	ILE	287	3.973	9.009	44.714
ATOM	2616	CG1	ILE	287	5.268	7.370	46.657
ATOM	2617	HG1	ILE	287	5.211	6.356	47.054
ATOM	2618	HG1	ILE	287	4.419	7.962	46.998
ATOM	2619	CD1	ILE	287	6.536	8.015	47.203
ATOM	2620	HD1	ILE	287	6.495	8.033	48.292
ATOM	2621	HD1	ILE	287	7.405	7.439	46.882
ATOM	2622	HD1	ILE	287	6.617	9.034	46.825
ATOM	2623	C	ILE	287	2.824	6.878	45.004
ATOM	2624	O	ILE	287	2.349	7.780	44.316
ATOM	2625	N	PHE	288	2.166	6.336	46.041
ATOM	2626	HN	PHE	288	2.619	5.606	46.610
ATOM	2627	CA	PHE	288	0.844	6.766	46.360
ATOM	2628	HA	PHE	288	0.314	7.005	45.438
ATOM	2629	CB	PHE	288	0.022	5.701	47.109
ATOM	2630	HB1	PHE	288	-0.024	4.814	46.477
ATOM	2631	HB2	PHE	288	-0.972	6.113	47.284
ATOM	2632	CG	PHE	288	0.719	5.411	48.394
ATOM	2633	CD1	PHE	288	0.473	6.170	49.516
ATOM	2634	HD1	PHE	288	-0.239	6.993	49.465
ATOM	2635	CD2	PHE	288	1.622	4.377	48.476
ATOM	2636	HD2	PHE	288	1.825	3.768	47.596
ATOM	2637	CE1	PHE	288	1.118	5.902	50.700
ATOM	2638	HE1	PHE	288	0.915	6.510	51.581
ATOM	2639	CE2	PHE	288	2.271	4.104	49.658
ATOM	2640	HE2	PHE	288	2.985	3.282	49.710
ATOM	2641	CZ	PHE	288	2.019	4.867	50.772
ATOM	2642	HZ	PHE	288	2.532	4.652	51.710
ATOM	2643	C	PHE	288	0.919	7.975	47.226
ATOM	2644	O	PHE	288	1.985	8.365	47.700
ATOM	2645	N	GLY	289	-0.246	8.614	47.413
ATOM	2646	HN	GLY	289	-1.081	8.270	46.918
ATOM	2647	CA	GLY	289	-0.380	9.751	48.268
ATOM	2648	HA1	GLY	289	-0.452	10.594	47.581
ATOM	2649	HA2	GLY	289	0.528	9.741	48.870
ATOM	2650	C	GLY	289	-1.627	9.482	49.039
ATOM	2651	O	GLY	289	-2.633	9.061	48.474
ATOM	2652	N	GLY	290	-1.623	9.766	50.352
ATOM	2653	HN	GLY	290	-0.809	10.219	50.793
ATOM	2654	CA	GLY	290	-2.781	9.422	51.122
ATOM	2655	HA1	GLY	290	-2.987	8.367	50.938
ATOM	2656	HA2	GLY	290	-3.596	10.058	50.777
ATOM	2657	C	GLY	290	-2.450	9.676	52.550
ATOM	2658	O	GLY	290	-3.336	9.797	53.394
ATOM	2659	N	THR	291	-1.144	9.740	52.861
ATOM	2660	HN	THR	291	-0.430	9.564	52.140

ATOM	2661	CA	THR	291	-0.752	10.053	54.200
ATOM	2662	HA	THR	291	-1.670	10.259	54.751
ATOM	2663	CB	THR	291	0.034	8.963	54.865
ATOM	2664	HB	THR	291	-0.531	8.034	54.798
ATOM	2665	OG1	THR	291	0.239	9.270	56.236
ATOM	2666	HG1	THR	291	0.690	10.193	56.318
ATOM	2667	CG2	THR	291	1.384	8.819	54.141
ATOM	2668	HG2	THR	291	1.968	8.029	54.615
ATOM	2669	HG2	THR	291	1.211	8.565	53.096
ATOM	2670	HG2	THR	291	1.931	9.760	54.201
ATOM	2671	C	THR	291	0.135	11.249	54.113
ATOM	2672	O	THR	291	0.847	11.440	53.129
ATOM	2673	N	PRO	292	0.076	12.091	55.104
ATOM	2674	CA	PRO	292	0.963	13.219	55.127
ATOM	2675	HA	PRO	292	0.975	13.613	54.111
ATOM	2676	CD	PRO	292	-1.165	12.363	55.802
ATOM	2677	HD1	PRO	292	-1.532	11.470	56.306
ATOM	2678	HD2	PRO	292	-1.937	12.699	55.109
ATOM	2679	CB	PRO	292	0.343	14.234	56.091
ATOM	2680	HB1	PRO	292	-0.012	15.042	55.452
ATOM	2681	HB2	PRO	292	1.160	14.526	56.751
ATOM	2682	CG	PRO	292	-0.784	13.464	56.803
ATOM	2683	HG1	PRO	292	-1.627	14.120	57.018
ATOM	2684	HG2	PRO	292	-0.433	13.045	57.746
ATOM	2685	C	PRO	292	2.291	12.689	55.553
ATOM	2686	O	PRO	292	2.312	11.692	56.272
ATOM	2687	N	THR	293	3.410	13.304	55.125
ATOM	2688	HN	THR	293	3.372	14.144	54.530
ATOM	2689	CA	THR	293	4.657	12.730	55.540
ATOM	2690	HA	THR	293	4.615	12.530	56.611
ATOM	2691	CB	THR	293	4.965	11.443	54.826
ATOM	2692	HB	THR	293	4.086	10.800	54.875
ATOM	2693	OG1	THR	293	6.043	10.762	55.450
ATOM	2694	HG1	THR	293	5.950	10.837	56.473
ATOM	2695	CG2	THR	293	5.310	11.768	53.361
ATOM	2696	HG2	THR	293	5.537	10.845	52.828
ATOM	2697	HG2	THR	293	4.462	12.261	52.888
ATOM	2698	HG2	THR	293	6.178	12.427	53.330
ATOM	2699	C	THR	293	5.760	13.698	55.243
ATOM	2700	O	THR	293	5.512	14.853	54.898
ATOM	2701	N	GLN	294	7.018	13.232	55.407
ATOM	2702	HN	GLN	294	7.145	12.267	55.745
ATOM	2703	CA	GLN	294	8.185	14.020	55.132
ATOM	2704	HA	GLN	294	7.953	15.029	55.474
ATOM	2705	CB	GLN	294	9.463	13.495	55.808
ATOM	2706	HB1	GLN	294	9.376	13.399	56.890
ATOM	2707	HB2	GLN	294	10.333	14.131	55.649
ATOM	2708	CG	GLN	294	9.889	12.109	55.319
ATOM	2709	HG1	GLN	294	10.886	11.901	55.706
ATOM	2710	HG2	GLN	294	9.894	12.118	54.229
ATOM	2711	CD	GLN	294	8.888	11.089	55.842
ATOM	2712	OE1	GLN	294	8.171	11.339	56.810
ATOM	2713	NE2	GLN	294	8.837	9.900	55.184
ATOM	2714	HE2	GLN	294	9.455	9.730	54.378
ATOM	2715	HE2	GLN	294	8.182	9.168	55.493
ATOM	2716	C	GLN	294	8.393	13.945	53.656
ATOM	2717	O	GLN	294	8.364	12.866	53.071
ATOM	2718	N	VAL	295	8.607	15.117	53.030
ATOM	2719	HN	VAL	295	8.702	15.963	53.609
ATOM	2720	CA	VAL	295	8.711	15.261	51.607
ATOM	2721	HA	VAL	295	7.868	14.803	51.090
ATOM	2722	CB	VAL	295	8.762	16.700	51.190
ATOM	2723	HB	VAL	295	8.832	16.741	50.103
ATOM	2724	CG1	VAL	295	7.476	17.390	51.674
ATOM	2725	HG1	VAL	295	7.494	18.440	51.380
ATOM	2726	HG1	VAL	295	6.610	16.903	51.226
ATOM	2727	HG1	VAL	295	7.411	17.319	52.760
ATOM	2728	CG2	VAL	295	10.060	17.321	51.733

ATOM	2729	HG2	VAL	295	10.113	18.369	51.438
ATOM	2730	HG2	VAL	295	10.071	17.249	52.820
ATOM	2731	HG2	VAL	295	10.918	16.786	51.325
ATOM	2732	C	VAL	295	9.952	14.621	51.071
ATOM	2733	O	VAL	295	9.928	14.073	49.970
ATOM	2734	N	LEU	296	11.061	14.679	51.836
ATOM	2735	HN	LEU	296	10.977	15.056	52.791
ATOM	2736	CA	LEU	296	12.356	14.241	51.387
ATOM	2737	HA	LEU	296	12.801	14.943	50.682
ATOM	2738	CB	LEU	296	13.389	14.119	52.522
ATOM	2739	HB1	LEU	296	14.351	13.722	52.197
ATOM	2740	HB2	LEU	296	13.072	13.461	53.332
ATOM	2741	CG	LEU	296	13.720	15.459	53.203
ATOM	2742	HG	LEU	296	14.068	16.197	52.480
ATOM	2743	CD2	LEU	296	14.932	15.326	54.138
ATOM	2744	HD2	LEU	296	15.140	16.289	54.604
ATOM	2745	HD2	LEU	296	14.716	14.588	54.911
ATOM	2746	HD2	LEU	296	15.801	15.005	53.563
ATOM	2747	CD1	LEU	296	12.487	16.049	53.908
ATOM	2748	HD1	LEU	296	12.754	16.995	54.379
ATOM	2749	HD1	LEU	296	11.696	16.218	53.177
ATOM	2750	HD1	LEU	296	12.135	15.352	54.669
ATOM	2751	C	LEU	296	12.289	12.915	50.698
ATOM	2752	O	LEU	296	12.052	11.878	51.315
ATOM	2753	N	ASN	297	12.493	12.954	49.365
ATOM	2754	HN	ASN	297	12.601	13.882	48.932
ATOM	2755	CA	ASN	297	12.572	11.812	48.500
ATOM	2756	HA	ASN	297	12.864	12.120	47.496
ATOM	2757	CB	ASN	297	13.619	10.787	48.968
ATOM	2758	HB1	ASN	297	13.208	10.221	49.805
ATOM	2759	HB2	ASN	297	14.517	11.319	49.280
ATOM	2760	CG	ASN	297	13.941	9.849	47.810
ATOM	2761	OD1	ASN	297	13.408	9.981	46.709
ATOM	2762	ND2	ASN	297	14.848	8.869	48.066
ATOM	2763	HD2	ASN	297	15.272	8.792	49.001
ATOM	2764	HD2	ASN	297	15.110	8.204	47.324
ATOM	2765	C	ASN	297	11.243	11.128	48.424
ATOM	2766	O	ASN	297	11.045	10.241	47.596
ATOM	2767	N	ILE	298	10.283	11.522	49.278
ATOM	2768	HN	ILE	298	10.459	12.282	49.951
ATOM	2769	CA	ILE	298	9.011	10.864	49.235
ATOM	2770	HA	ILE	298	9.169	9.787	49.194
ATOM	2771	CB	ILE	298	8.166	11.120	50.462
ATOM	2772	HB	ILE	298	8.772	10.947	51.352
ATOM	2773	CG2	ILE	298	7.674	12.576	50.436
ATOM	2774	HG2	ILE	298	7.063	12.770	51.318
ATOM	2775	HG2	ILE	298	8.532	13.249	50.434
ATOM	2776	HG2	ILE	298	7.079	12.743	49.538
ATOM	2777	CG1	ILE	298	7.023	10.091	50.579
ATOM	2778	HG1	ILE	298	6.505	10.266	51.522
ATOM	2779	HG1	ILE	298	7.461	9.093	50.557
ATOM	2780	CD1	ILE	298	5.981	10.159	49.463
ATOM	2781	HD1	ILE	298	5.218	9.399	49.631
ATOM	2782	HD1	ILE	298	5.516	11.145	49.459
ATOM	2783	HD1	ILE	298	6.464	9.982	48.503
ATOM	2784	C	ILE	298	8.268	11.317	48.015
ATOM	2785	O	ILE	298	7.655	10.512	47.318
ATOM	2786	N	THR	299	8.326	12.625	47.699
ATOM	2787	HN	THR	299	8.932	13.260	48.239
ATOM	2788	CA	THR	299	7.543	13.133	46.612
ATOM	2789	HA	THR	299	7.026	12.300	46.136
ATOM	2790	CB	THR	299	6.540	14.152	47.052
ATOM	2791	HB	THR	299	5.923	13.701	47.829
ATOM	2792	OG1	THR	299	5.705	14.530	45.967
ATOM	2793	HG1	THR	299	5.593	15.554	45.960
ATOM	2794	CG2	THR	299	7.308	15.365	47.594
ATOM	2795	HG2	THR	299	6.601	16.126	47.923
ATOM	2796	HG2	THR	299	7.927	15.057	48.436

ATOM	2797	HG2	THR	299	7.943	15.775	46.808
ATOM	2798	C	THR	299	8.453	13.799	45.641
ATOM	2799	O	THR	299	9.616	14.067	45.944
ATOM	2800	N	GLN	300	7.940	14.078	44.424
ATOM	2801	HN	GLN	300	6.954	13.873	44.208
ATOM	2802	CA	GLN	300	8.798	14.664	43.443
ATOM	2803	HA	GLN	300	9.843	14.430	43.644
ATOM	2804	CB	GLN	300	8.600	14.163	42.000
ATOM	2805	HB1	GLN	300	8.658	13.074	42.010
ATOM	2806	HB2	GLN	300	9.392	14.588	41.384
ATOM	2807	CG	GLN	300	7.269	14.540	41.353
ATOM	2808	HG1	GLN	300	7.148	15.613	41.499
ATOM	2809	HG2	GLN	300	6.501	13.963	41.869
ATOM	2810	CD	GLN	300	7.383	14.165	39.881
ATOM	2811	OE1	GLN	300	7.435	12.990	39.523
ATOM	2812	NE2	GLN	300	7.444	15.195	38.996
ATOM	2813	HE2	GLN	300	7.397	16.167	39.333
ATOM	2814	HE2	GLN	300	7.538	15.003	37.988
ATOM	2815	C	GLN	300	8.658	16.155	43.425
ATOM	2816	O	GLN	300	8.025	16.768	44.283
ATOM	2817	N	GLU	301	9.270	16.740	42.379
ATOM	2818	HN	GLU	301	9.648	16.088	41.676
ATOM	2819	CA	GLU	301	9.479	18.131	42.090
ATOM	2820	HA	GLU	301	9.979	18.671	42.894
ATOM	2821	CB	GLU	301	10.342	18.329	40.834
ATOM	2822	HB1	GLU	301	10.429	19.398	40.641
ATOM	2823	HB2	GLU	301	9.852	17.829	39.998
ATOM	2824	CG	GLU	301	11.754	17.760	40.955
ATOM	2825	HG1	GLU	301	12.122	17.992	41.955
ATOM	2826	HG2	GLU	301	12.370	18.232	40.190
ATOM	2827	CD	GLU	301	11.669	16.254	40.738
ATOM	2828	OE1	GLU	301	10.579	15.781	40.319
ATOM	2829	OE2	GLU	301	12.691	15.560	40.985
ATOM	2831	C	GLU	301	8.209	18.886	41.841
ATOM	2832	O	GLU	301	8.164	20.095	42.059
ATOM	2833	N	CYS	302	7.142	18.209	41.388
ATOM	2834	HN	CYS	302	7.164	17.180	41.372
ATOM	2835	CA	CYS	302	5.968	18.897	40.924
ATOM	2836	HA	CYS	302	6.126	19.452	39.999
ATOM	2837	CB	CYS	302	4.808	17.953	40.565
ATOM	2838	HB1	CYS	302	3.865	18.485	40.438
ATOM	2839	HB2	CYS	302	4.636	17.198	41.332
ATOM	2840	SG	CYS	302	5.104	17.053	39.014
ATOM	2841	HG	CYS	302	4.320	17.554	38.049
ATOM	2842	C	CYS	302	5.435	19.912	41.907
ATOM	2843	O	CYS	302	4.999	20.973	41.470
ATOM	2844	N	PHE	303	5.435	19.679	43.238
ATOM	2845	HN	PHE	303	5.871	18.836	43.638
ATOM	2846	CA	PHE	303	4.793	20.669	44.072
ATOM	2847	HA	PHE	303	3.947	21.131	43.564
ATOM	2848	CB	PHE	303	4.165	20.088	45.354
ATOM	2849	HB1	PHE	303	4.971	19.862	46.052
ATOM	2850	HB2	PHE	303	3.621	19.183	45.082
ATOM	2851	CG	PHE	303	3.242	21.113	45.921
ATOM	2852	CD1	PHE	303	2.002	21.321	45.360
ATOM	2853	HD1	PHE	303	1.699	20.734	44.493
ATOM	2854	CD2	PHE	303	3.602	21.857	47.020
ATOM	2855	HD2	PHE	303	4.576	21.700	47.481
ATOM	2856	CE1	PHE	303	1.141	22.260	45.878
ATOM	2857	HE1	PHE	303	0.164	22.415	45.420
ATOM	2858	CE2	PHE	303	2.745	22.798	47.543
ATOM	2859	HE2	PHE	303	3.045	23.382	48.413
ATOM	2860	CZ	PHE	303	1.512	23.003	46.972
ATOM	2861	HZ	PHE	303	0.834	23.750	47.385
ATOM	2862	C	PHE	303	5.742	21.766	44.450
ATOM	2863	O	PHE	303	6.717	21.578	45.178
ATOM	2864	N	LYS	304	5.433	22.985	43.975
ATOM	2865	HN	LYS	304	4.581	23.107	43.409

ATOM	2866	CA	LYS	304	6.268	24.113	44.242
ATOM	2867	HA	LYS	304	7.253	23.919	43.816
ATOM	2868	CB	LYS	304	5.737	25.406	43.588
ATOM	2869	HB1	LYS	304	5.896	25.330	42.512
ATOM	2870	HB2	LYS	304	6.292	26.247	44.004
ATOM	2871	CG	LYS	304	4.245	25.690	43.809
ATOM	2872	HG1	LYS	304	3.698	24.760	43.657
ATOM	2873	HG2	LYS	304	3.935	26.445	43.086
ATOM	2874	CD	LYS	304	3.878	26.212	45.198
ATOM	2875	HD1	LYS	304	4.366	27.153	45.455
ATOM	2876	HD2	LYS	304	4.140	25.529	46.006
ATOM	2877	CE	LYS	304	2.382	26.481	45.378
ATOM	2878	HE1	LYS	304	1.815	25.565	45.212
ATOM	2879	HE2	LYS	304	2.050	27.236	44.665
ATOM	2880	NZ	LYS	304	2.117	26.967	46.751
ATOM	2881	HZ1	LYS	304	1.109	27.146	46.864
ATOM	2882	HZ2	LYS	304	2.417	26.255	47.432
ATOM	2883	HZ3	LYS	304	2.640	27.840	46.913
ATOM	2884	C	LYS	304	6.361	24.287	45.721
ATOM	2885	O	LYS	304	7.430	24.585	46.251
ATOM	2886	N	GLY	305	5.246	24.082	46.441
ATOM	2887	HN	GLY	305	4.371	23.802	45.976
ATOM	2888	CA	GLY	305	5.288	24.257	47.860
ATOM	2889	HA1	GLY	305	6.252	23.857	48.172
ATOM	2890	HA2	GLY	305	4.441	23.690	48.245
ATOM	2891	C	GLY	305	5.161	25.719	48.079
ATOM	2892	O	GLY	305	5.651	26.503	47.268
ATOM	2893	N	ILE	306	4.501	26.118	49.184
ATOM	2894	HN	ILE	306	4.123	25.418	49.838
ATOM	2895	CA	ILE	306	4.326	27.513	49.449
ATOM	2896	HA	ILE	306	3.697	27.920	48.658
ATOM	2897	CB	ILE	306	3.594	27.798	50.731
ATOM	2898	HB	ILE	306	3.598	28.878	50.880
ATOM	2899	CG2	ILE	306	2.161	27.263	50.578
ATOM	2900	HG2	ILE	306	1.601	27.454	51.493
ATOM	2901	HG2	ILE	306	1.673	27.764	49.742
ATOM	2902	HG2	ILE	306	2.191	26.190	50.389
ATOM	2903	CG1	ILE	306	4.337	27.222	51.943
ATOM	2904	HG1	ILE	306	5.393	27.492	51.966
ATOM	2905	HG1	ILE	306	4.312	26.133	51.983
ATOM	2906	CD1	ILE	306	3.763	27.695	53.279
ATOM	2907	HD1	ILE	306	4.333	27.252	54.096
ATOM	2908	HD1	ILE	306	3.828	28.781	53.338
ATOM	2909	HD1	ILE	306	2.720	27.389	53.356
ATOM	2910	C	ILE	306	5.674	28.141	49.449
ATOM	2911	O	ILE	306	6.478	27.978	50.364
ATOM	2912	N	LEU	307	5.941	28.867	48.354
ATOM	2913	HN	LEU	307	5.192	28.985	47.656
ATOM	2914	CA	LEU	307	7.199	29.486	48.098
ATOM	2915	HA	LEU	307	7.955	28.703	48.134
ATOM	2916	CB	LEU	307	7.210	30.189	46.725
ATOM	2917	HB1	LEU	307	6.423	30.943	46.727
ATOM	2918	HB2	LEU	307	7.025	29.435	45.960
ATOM	2919	CG	LEU	307	8.523	30.905	46.351
ATOM	2920	HG	LEU	307	8.558	31.200	45.302
ATOM	2921	CD2	LEU	307	9.714	29.929	46.432
ATOM	2922	HD2	LEU	307	10.632	30.452	46.165
ATOM	2923	HD2	LEU	307	9.799	29.543	47.448
ATOM	2924	HD2	LEU	307	9.554	29.101	45.742
ATOM	2925	CD1	LEU	307	8.750	32.186	47.158
ATOM	2926	HD1	LEU	307	9.689	32.648	46.853
ATOM	2927	HD1	LEU	307	7.929	32.880	46.977
ATOM	2928	HD1	LEU	307	8.793	31.944	48.220
ATOM	2929	C	LEU	307	7.410	30.505	49.163
ATOM	2930	O	LEU	307	8.534	30.723	49.608
ATOM	2931	N	LYS	308	6.319	31.148	49.609
ATOM	2932	HN	LYS	308	5.382	30.859	49.292
ATOM	2933	CA	LYS	308	6.463	32.233	50.524

ATOM	2934	HA	LYS	308	7.048	33.047	50.097
ATOM	2935	CB	LYS	308	5.116	32.858	50.931
ATOM	2936	HB1	LYS	308	4.471	32.172	51.481
ATOM	2937	HB2	LYS	308	4.524	33.195	50.080
ATOM	2938	CG	LYS	308	5.268	34.086	51.833
ATOM	2939	HG1	LYS	308	6.044	34.727	51.414
ATOM	2940	HG2	LYS	308	5.550	33.747	52.830
ATOM	2941	CD	LYS	308	3.992	34.919	51.965
ATOM	2942	HD1	LYS	308	3.151	34.365	52.383
ATOM	2943	HD2	LYS	308	3.629	35.312	51.015
ATOM	2944	CE	LYS	308	4.151	36.144	52.868
ATOM	2945	HE1	LYS	308	4.925	36.802	52.473
ATOM	2946	HE2	LYS	308	4.433	35.833	53.874
ATOM	2947	NZ	LYS	308	2.877	36.893	52.939
ATOM	2948	HZ1	LYS	308	2.994	37.714	53.548
ATOM	2949	HZ2	LYS	308	2.607	37.202	51.994
ATOM	2950	HZ3	LYS	308	2.141	36.283	53.323
ATOM	2951	C	LYS	308	7.153	31.809	51.784
ATOM	2952	O	LYS	308	8.133	32.436	52.181
ATOM	2953	N	ASP	309	6.702	30.728	52.452
ATOM	2954	HN	ASP	309	5.948	30.131	52.082
ATOM	2955	CA	ASP	309	7.337	30.463	53.712
ATOM	2956	HA	ASP	309	7.338	31.351	54.345
ATOM	2957	CB	ASP	309	6.610	29.452	54.635
ATOM	2958	HB1	ASP	309	5.567	29.706	54.821
ATOM	2959	HB2	ASP	309	7.062	29.362	55.623
ATOM	2960	CG	ASP	309	6.582	28.034	54.079
ATOM	2961	OD1	ASP	309	6.841	27.841	52.864
ATOM	2962	OD2	ASP	309	6.287	27.111	54.884
ATOM	2963	C	ASP	309	8.760	30.037	53.518
ATOM	2964	O	ASP	309	9.643	30.454	54.266
ATOM	2965	N	LYS	310	9.026	29.208	52.494
ATOM	2966	HN	LYS	310	8.267	28.936	51.852
ATOM	2967	CA	LYS	310	10.346	28.697	52.280
ATOM	2968	HA	LYS	310	10.683	28.199	53.189
ATOM	2969	CB	LYS	310	10.370	27.637	51.162
ATOM	2970	HB1	LYS	310	9.775	26.784	51.487
ATOM	2971	HB2	LYS	310	11.406	27.342	50.994
ATOM	2972	CG	LYS	310	9.802	28.114	49.824
ATOM	2973	HG1	LYS	310	8.928	28.757	49.921
ATOM	2974	HG2	LYS	310	9.482	27.304	49.169
ATOM	2975	CD	LYS	310	10.790	28.923	48.989
ATOM	2976	HD1	LYS	310	11.586	29.351	49.598
ATOM	2977	HD2	LYS	310	10.306	29.753	48.474
ATOM	2978	CE	LYS	310	11.465	28.072	47.916
ATOM	2979	HE1	LYS	310	12.233	28.655	47.407
ATOM	2980	HE2	LYS	310	10.727	27.742	47.184
ATOM	2981	NZ	LYS	310	12.094	26.882	48.535
ATOM	2982	HZ1	LYS	310	12.547	26.314	47.806
ATOM	2983	HZ2	LYS	310	12.800	27.185	49.222
ATOM	2984	HZ3	LYS	310	11.373	26.320	49.010
ATOM	2985	C	LYS	310	11.256	29.834	51.951
ATOM	2986	O	LYS	310	12.376	29.917	52.454
ATOM	2987	N	LYS	311	10.771	30.770	51.125
ATOM	2988	HN	LYS	311	9.806	30.685	50.773
ATOM	2989	CA	LYS	311	11.571	31.885	50.723
ATOM	2990	HA	LYS	311	12.472	31.502	50.245
ATOM	2991	CB	LYS	311	10.833	32.824	49.750
ATOM	2992	HB1	LYS	311	9.923	33.258	50.163
ATOM	2993	HB2	LYS	311	10.517	32.340	48.826
ATOM	2994	CG	LYS	311	11.668	34.024	49.298
ATOM	2995	HG1	LYS	311	12.675	33.754	48.979
ATOM	2996	HG2	LYS	311	11.804	34.774	50.076
ATOM	2997	CD	LYS	311	11.058	34.776	48.114
ATOM	2998	HD1	LYS	311	10.065	35.179	48.317
ATOM	2999	HD2	LYS	311	10.935	34.162	47.222
ATOM	3000	CE	LYS	311	11.886	35.977	47.657
ATOM	3001	HE1	LYS	311	12.880	35.649	47.350

```
ATOM   3002  HE2 LYS   311      11.986  36.693  48.472
ATOM   3003  NZ  LYS   311      11.225  36.641  46.512
ATOM   3004  HZ1 LYS   311      11.789  37.448  46.210
ATOM   3005  HZ2 LYS   311      11.135  35.974  45.732
ATOM   3006  HZ3 LYS   311      10.289  36.964  46.795
ATOM   3007  C   LYS   311      11.913  32.675  51.940
ATOM   3008  O   LYS   311      13.005  33.229  52.047
ATOM   3009  N   ASN   312      10.984  32.755  52.905
ATOM   3010  HN  ASN   312      10.097  32.239  52.827
ATOM   3011  CA  ASN   312      11.257  33.575  54.045
ATOM   3012  HA  ASN   312      11.420  34.609  53.739
ATOM   3013  CB  ASN   312      10.099  33.574  55.063
ATOM   3014  HB1 ASN   312      10.036  32.590  55.527
ATOM   3015  HB2 ASN   312       9.168  33.801  54.542
ATOM   3016  CG  ASN   312      10.372  34.633  56.125
ATOM   3017  OD1 ASN   312      11.435  34.669  56.741
ATOM   3018  ND2 ASN   312       9.373  35.531  56.346
ATOM   3019  HD2 ASN   312       8.496  35.468  55.809
ATOM   3020  HD2 ASN   312       9.495  36.273  57.050
ATOM   3021  C   ASN   312      12.484  33.089  54.758
ATOM   3022  O   ASN   312      13.420  33.856  54.976
ATOM   3023  N   ASP   313      12.519  31.797  55.141
ATOM   3024  HN  ASP   313      11.753  31.159  54.884
ATOM   3025  CA  ASP   313      13.633  31.317  55.912
ATOM   3026  HA  ASP   313      13.846  31.958  56.767
ATOM   3027  CB  ASP   313      13.389  29.912  56.491
ATOM   3028  HB1 ASP   313      13.397  29.191  55.674
ATOM   3029  HB2 ASP   313      12.421  29.904  56.992
ATOM   3030  CG  ASP   313      14.499  29.594  57.485
ATOM   3031  OD1 ASP   313      15.396  30.458  57.678
ATOM   3032  OD2 ASP   313      14.459  28.480  58.071
ATOM   3033  C   ASP   313      14.893  31.247  55.098
ATOM   3034  O   ASP   313      15.914  31.818  55.477
ATOM   3035  N   ILE   314      14.840  30.543  53.951
ATOM   3036  HN  ILE   314      13.931  30.171  53.642
ATOM   3037  CA  ILE   314      16.001  30.290  53.140
ATOM   3038  HA  ILE   314      16.848  29.957  53.740
ATOM   3039  CB  ILE   314      15.818  29.155  52.172
ATOM   3040  HB  ILE   314      16.744  29.065  51.605
ATOM   3041  CG2 ILE   314      15.534  27.894  53.003
ATOM   3042  HG2 ILE   314      15.394  27.043  52.337
ATOM   3043  HG2 ILE   314      16.375  27.699  53.668
ATOM   3044  HG2 ILE   314      14.631  28.044  53.595
ATOM   3045  CG1 ILE   314      14.731  29.445  51.128
ATOM   3046  HG1 ILE   314      14.891  30.396  50.619
ATOM   3047  HG1 ILE   314      13.736  29.494  51.571
ATOM   3048  CD1 ILE   314      14.672  28.373  50.041
ATOM   3049  HD1 ILE   314      13.888  28.623  49.326
ATOM   3050  HD1 ILE   314      15.631  28.325  49.525
ATOM   3051  HD1 ILE   314      14.455  27.406  50.494
ATOM   3052  C   ILE   314      16.439  31.514  52.401
ATOM   3053  O   ILE   314      17.616  31.642  52.065
ATOM   3054  N   GLU   315      15.488  32.421  52.112
ATOM   3055  HN  GLU   315      14.538  32.218  52.456
ATOM   3056  CA  GLU   315      15.658  33.644  51.373
ATOM   3057  HA  GLU   315      14.725  34.208  51.379
ATOM   3058  CB  GLU   315      16.633  34.692  51.965
ATOM   3059  HB1 GLU   315      16.327  34.881  52.993
ATOM   3060  HB2 GLU   315      16.556  35.593  51.355
ATOM   3061  CG  GLU   315      18.119  34.328  52.014
ATOM   3062  HG1 GLU   315      18.700  35.213  51.754
ATOM   3063  HG2 GLU   315      18.302  33.528  51.297
ATOM   3064  CD  GLU   315      18.455  33.866  53.426
ATOM   3065  OE1 GLU   315      17.508  33.744  54.248
ATOM   3066  OE2 GLU   315      19.662  33.627  53.700
ATOM   3068  C   GLU   315      16.035  33.328  49.964
ATOM   3069  O   GLU   315      16.677  34.123  49.280
ATOM   3070  N   ALA   316      15.620  32.138  49.494
```

	ATOM	3071	HN	ALA	316	15.141	31.488	50.133
	ATOM	3072	CA	ALA	316	15.825	31.747	48.134
	ATOM	3073	HA	ALA	316	15.932	32.684	47.588
	ATOM	3074	CB	ALA	316	17.028	30.811	47.931
5	ATOM	3075	HB1	ALA	316	17.118	30.559	46.874
	ATOM	3076	HB2	ALA	316	17.938	31.311	48.264
	ATOM	3077	HB3	ALA	316	16.882	29.899	48.510
	ATOM	3078	C	ALA	316	14.602	30.978	47.770
	ATOM	3079	O	ALA	316	13.837	30.575	48.642
10	ATOM	3080	N	GLN	317	14.355	30.790	46.464
	ATOM	3081	HN	GLN	317	14.951	31.225	45.745
	ATOM	3082	CA	GLN	317	13.244	29.970	46.096
	ATOM	3083	HA	GLN	317	12.404	30.119	46.774
	ATOM	3084	CB	GLN	317	12.787	30.170	44.639
15	ATOM	3085	HB1	GLN	317	13.561	29.940	43.907
	ATOM	3086	HB2	GLN	317	12.478	31.191	44.418
	ATOM	3087	CG	GLN	317	11.592	29.294	44.250
	ATOM	3088	HG1	GLN	317	10.703	29.682	44.748
	ATOM	3089	HG2	GLN	317	11.793	28.272	44.571
20	ATOM	3090	CD	GLN	317	11.423	29.353	42.741
	ATOM	3091	OE1	GLN	317	12.182	30.026	42.045
	ATOM	3092	NE2	GLN	317	10.406	28.615	42.219
	ATOM	3093	HE2	GLN	317	9.796	28.067	42.841
	ATOM	3094	HE2	GLN	317	10.246	28.605	41.201
25	ATOM	3095	C	GLN	317	13.799	28.597	46.193
	ATOM	3096	O	GLN	317	14.136	28.135	47.282
	ATOM	3097	N	TRP	318	13.907	27.901	45.049
	ATOM	3098	HN	TRP	318	13.524	28.260	44.162
	ATOM	3099	CA	TRP	318	14.574	26.649	45.118
30	ATOM	3100	HA	TRP	318	14.080	25.983	45.826
	ATOM	3101	CB	TRP	318	14.701	25.917	43.774
	ATOM	3102	HB1	TRP	318	15.480	25.159	43.868
	ATOM	3103	HB2	TRP	318	14.968	26.645	43.009
	ATOM	3104	CG	TRP	318	13.438	25.227	43.334
35	ATOM	3105	CD2	TRP	318	13.213	23.824	43.520
	ATOM	3106	CD1	TRP	318	12.327	25.721	42.716
	ATOM	3107	HD1	TRP	318	12.181	26.762	42.428
	ATOM	3108	NE1	TRP	318	11.419	24.709	42.511
	ATOM	3109	HE1	TRP	318	10.496	24.810	42.066
40	ATOM	3110	CE2	TRP	318	11.953	23.535	43.000
	ATOM	3111	CE3	TRP	318	13.992	22.855	44.083
	ATOM	3112	HE3	TRP	318	14.976	23.084	44.492
	ATOM	3113	CZ2	TRP	318	11.450	22.267	43.040
	ATOM	3114	HZ2	TRP	318	10.461	22.038	42.642
45	ATOM	3115	CZ3	TRP	318	13.484	21.576	44.113
	ATOM	3116	HZ3	TRP	318	14.080	20.775	44.550
	ATOM	3117	CH2	TRP	318	12.237	21.287	43.602
	ATOM	3118	HH2	TRP	318	11.867	20.263	43.643
	ATOM	3119	C	TRP	318	15.934	27.003	45.561
50	ATOM	3120	O	TRP	318	16.704	27.633	44.839
	ATOM	3121	N	HIS	319	16.265	26.644	46.804
	ATOM	3122	HN	HIS	319	15.590	26.209	47.449
	ATOM	3123	CA	HIS	319	17.609	26.903	47.178
	ATOM	3124	HA	HIS	319	17.968	27.836	46.744
55	ATOM	3125	ND1	HIS	319	19.405	28.897	49.152
	ATOM	3126	HD1	HIS	319	18.737	29.653	48.947
	ATOM	3127	CG	HIS	319	19.158	27.543	49.089
	ATOM	3128	NE2	HIS	319	21.298	27.881	49.725
	ATOM	3129	HE2	HIS	319	22.271	27.714	50.017
60	ATOM	3130	CD2	HIS	319	20.325	26.938	49.441
	ATOM	3131	HD2	HIS	319	20.474	25.860	49.493
	ATOM	3132	CE1	HIS	319	20.698	29.042	49.537
	ATOM	3133	HE1	HIS	319	21.186	30.007	49.675
	ATOM	3134	CB	HIS	319	17.831	26.955	48.701
65	ATOM	3135	HB1	HIS	319	17.801	25.974	49.176
	ATOM	3136	HB2	HIS	319	17.086	27.553	49.226
	ATOM	3137	C	HIS	319	18.318	25.721	46.634
	ATOM	3138	O	HIS	319	17.970	25.193	45.578

ATOM	3139	N	ASP	320	19.339	25.255	47.343
ATOM	3140	HN	ASP	320	19.651	25.725	48.205
ATOM	3141	CA	ASP	320	19.985	24.084	46.866
ATOM	3142	HA	ASP	320	20.748	23.809	47.594
ATOM	3143	CB	ASP	320	19.014	22.906	46.680
ATOM	3144	HB1	ASP	320	18.406	23.133	45.804
ATOM	3145	HB2	ASP	320	18.414	22.844	47.588
ATOM	3146	CG	ASP	320	19.862	21.664	46.475
ATOM	3147	OD1	ASP	320	21.108	21.797	46.605
ATOM	3148	OD2	ASP	320	19.287	20.581	46.189
ATOM	3149	C	ASP	320	20.591	24.410	45.543
ATOM	3150	O	ASP	320	20.863	23.527	44.734
ATOM	3151	N	GLU	321	20.805	25.711	45.284
ATOM	3152	HN	GLU	321	20.507	26.433	45.956
ATOM	3153	CA	GLU	321	21.449	26.080	44.064
ATOM	3154	HA	GLU	321	20.858	25.621	43.272
ATOM	3155	CB	GLU	321	21.492	27.598	43.819
ATOM	3156	HB1	GLU	321	20.466	27.955	43.727
ATOM	3157	HB2	GLU	321	22.049	27.776	42.900
ATOM	3158	CG	GLU	321	22.160	28.416	44.920
ATOM	3159	HG1	GLU	321	23.186	28.056	44.997
ATOM	3160	HG2	GLU	321	21.591	28.234	45.832
ATOM	3161	CD	GLU	321	22.094	29.872	44.482
ATOM	3162	OE1	GLU	321	22.672	30.192	43.409
ATOM	3163	OE2	GLU	321	21.454	30.681	45.206
ATOM	3165	C	GLU	321	22.827	25.529	44.160
ATOM	3166	O	GLU	321	23.432	25.205	43.136
ATOM	3167	N	SER	322	23.347	25.443	45.412
ATOM	3168	HN	SER	322	22.814	25.829	46.204
ATOM	3169	CA	SER	322	24.618	24.827	45.659
ATOM	3170	HA	SER	322	25.430	25.437	45.262
ATOM	3171	CB	SER	322	24.927	24.624	47.160
ATOM	3172	HB1	SER	322	24.996	25.576	47.687
ATOM	3173	HB2	SER	322	25.872	24.103	47.309
ATOM	3174	OG	SER	322	23.918	23.859	47.803
ATOM	3175	HG	SER	322	23.260	24.491	48.282
ATOM	3176	C	SER	322	24.526	23.521	44.959
ATOM	3177	O	SER	322	25.115	23.387	43.897
ATOM	3178	N	HIS	323	23.752	22.560	45.498
ATOM	3179	HN	HIS	323	23.409	22.679	46.462
ATOM	3180	CA	HIS	323	23.388	21.374	44.775
ATOM	3181	HA	HIS	323	22.610	20.799	45.277
ATOM	3182	ND1	HIS	323	23.939	19.802	41.804
ATOM	3183	HD1	HIS	323	23.138	19.168	41.935
ATOM	3184	CG	HIS	323	24.093	21.047	42.361
ATOM	3185	NE2	HIS	323	25.895	20.563	41.076
ATOM	3186	HE2	HIS	323	26.802	20.635	40.593
ATOM	3187	CD2	HIS	323	25.298	21.496	41.902
ATOM	3188	HD2	HIS	323	25.732	22.463	42.154
ATOM	3189	CE1	HIS	323	25.041	19.562	41.048
ATOM	3190	HE1	HIS	323	25.200	18.644	40.481
ATOM	3191	CB	HIS	323	23.056	21.632	43.306
ATOM	3192	HB1	HIS	323	22.997	22.695	43.070
ATOM	3193	HB2	HIS	323	22.100	21.202	43.010
ATOM	3194	C	HIS	323	24.526	20.450	44.588
ATOM	3195	O	HIS	323	24.289	19.248	44.451
ATOM	3196	N	LEU	324	25.759	20.990	44.683
ATOM	3197	HN	LEU	324	25.853	21.886	45.182
ATOM	3198	CA	LEU	324	26.948	20.402	44.136
ATOM	3199	HA	LEU	324	26.967	20.551	43.057
ATOM	3200	CB	LEU	324	28.238	20.916	44.804
ATOM	3201	HB1	LEU	324	29.079	20.386	44.357
ATOM	3202	HB2	LEU	324	28.167	20.708	45.872
ATOM	3203	CG	LEU	324	28.526	22.420	44.658
ATOM	3204	HG	LEU	324	29.405	22.708	45.234
ATOM	3205	CD2	LEU	324	27.446	23.275	45.336
ATOM	3206	HD2	LEU	324	27.687	24.331	45.211
ATOM	3207	HD2	LEU	324	26.478	23.067	44.881

```
ATOM   3208  HD2 LEU   324      27.407  23.036  46.399
ATOM   3209  CD1 LEU   324      28.781  22.792  43.195
ATOM   3210  HD1 LEU   324      28.982  23.861  43.121
ATOM   3211  HD1 LEU   324      29.641  22.235  42.822
ATOM   3212  HD1 LEU   324      27.903  22.546  42.598
ATOM   3213  C   LEU   324      26.964  18.949  44.430
ATOM   3214  O   LEU   324      27.140  18.135  43.526
ATOM   3215  N   ASN   325      26.706  18.583  45.693
ATOM   3216  HN  ASN   325      26.480  19.291  46.406
ATOM   3217  CA  ASN   325      26.749  17.198  46.034
ATOM   3218  HA  ASN   325      27.658  16.729  45.657
ATOM   3219  CB  ASN   325      26.815  16.936  47.552
ATOM   3220  HB1 ASN   325      27.743  17.346  47.949
ATOM   3221  HB2 ASN   325      26.782  15.862  47.735
ATOM   3222  CG  ASN   325      25.629  17.606  48.231
ATOM   3223  OD1 ASN   325      24.608  16.987  48.528
ATOM   3224  ND2 ASN   325      25.786  18.928  48.504
ATOM   3225  HD2 ASN   325      26.658  19.409  48.238
ATOM   3226  HD2 ASN   325      25.034  19.450  48.976
ATOM   3227  C   ASN   325      25.583  16.464  45.452
ATOM   3228  O   ASN   325      25.266  16.592  44.272
ATOM   3229  N   LYS   326      24.918  15.656  46.293
ATOM   3230  HN  LYS   326      25.203  15.646  47.283
ATOM   3231  CA  LYS   326      23.836  14.806  45.892
ATOM   3232  HA  LYS   326      24.162  14.154  45.082
ATOM   3233  CB  LYS   326      23.320  13.917  47.038
ATOM   3234  HB1 LYS   326      22.934  14.484  47.885
ATOM   3235  HB2 LYS   326      24.085  13.262  47.456
ATOM   3236  CG  LYS   326      22.178  12.989  46.620
ATOM   3237  HG1 LYS   326      21.349  13.508  46.138
ATOM   3238  HG2 LYS   326      21.729  12.448  47.453
ATOM   3239  CD  LYS   326      22.604  11.907  45.625
ATOM   3240  HD1 LYS   326      23.383  11.245  46.004
ATOM   3241  HD2 LYS   326      23.002  12.303  44.691
ATOM   3242  CE  LYS   326      21.466  10.976  45.205
ATOM   3243  HE1 LYS   326      21.801  10.312  44.407
ATOM   3244  HE2 LYS   326      20.618  11.560  44.845
ATOM   3245  NZ  LYS   326      21.028  10.157  46.357
ATOM   3246  HZ1 LYS   326      20.262   9.534  46.064
ATOM   3247  HZ2 LYS   326      21.820   9.592  46.697
ATOM   3248  HZ3 LYS   326      20.699  10.775  47.112
ATOM   3249  C   LYS   326      22.690  15.639  45.423
ATOM   3250  O   LYS   326      21.808  15.145  44.722
ATOM   3251  N   TYR   327      22.680  16.933  45.786
ATOM   3252  HN  TYR   327      23.495  17.331  46.273
ATOM   3253  CA  TYR   327      21.549  17.763  45.504
ATOM   3254  HA  TYR   327      20.671  17.418  46.051
ATOM   3255  CB  TYR   327      21.740  19.220  45.934
ATOM   3256  HB1 TYR   327      20.870  19.767  45.570
ATOM   3257  HB2 TYR   327      22.666  19.561  45.471
ATOM   3258  CG  TYR   327      21.821  19.215  47.421
ATOM   3259  CD1 TYR   327      20.702  18.966  48.183
ATOM   3260  HD1 TYR   327      19.748  18.769  47.692
ATOM   3261  CD2 TYR   327      23.010  19.475  48.056
ATOM   3262  HD2 TYR   327      23.902  19.685  47.465
ATOM   3263  CE1 TYR   327      20.774  18.963  49.556
ATOM   3264  HE1 TYR   327      19.882  18.760  50.149
ATOM   3265  CE2 TYR   327      23.091  19.474  49.429
ATOM   3266  HE2 TYR   327      24.043  19.678  49.920
ATOM   3267  CZ  TYR   327      21.972  19.216  50.182
ATOM   3268  OH  TYR   327      22.050  19.213  51.590
ATOM   3269  HH  TYR   327      22.273  20.162  51.924
ATOM   3270  C   TYR   327      21.228  17.742  44.049
ATOM   3271  O   TYR   327      20.066  17.901  43.680
ATOM   3272  N   PHE   328      22.233  17.554  43.175
ATOM   3273  HN  PHE   328      23.201  17.416  43.497
ATOM   3274  CA  PHE   328      21.907  17.554  41.779
ATOM   3275  HA  PHE   328      21.453  18.518  41.551
```

ATOM	3276	CB	PHE	328	23.092	17.255	40.855
ATOM	3277	HB1	PHE	328	23.318	16.194	40.961
ATOM	3278	HB2	PHE	328	23.920	17.881	41.188
ATOM	3279	CG	PHE	328	22.659	17.596	39.469
ATOM	3280	CD1	PHE	328	21.861	16.738	38.747
ATOM	3281	HD1	PHE	328	21.540	15.796	39.191
ATOM	3282	CD2	PHE	328	23.059	18.779	38.889
ATOM	3283	HD2	PHE	328	23.694	19.465	39.449
ATOM	3284	CE1	PHE	328	21.466	17.060	37.470
ATOM	3285	HE1	PHE	328	20.832	16.374	36.908
ATOM	3286	CE2	PHE	328	22.666	19.106	37.613
ATOM	3287	HE2	PHE	328	22.989	20.047	37.167
ATOM	3288	CZ	PHE	328	21.867	18.245	36.900
ATOM	3289	HZ	PHE	328	21.553	18.500	35.887
ATOM	3290	C	PHE	328	20.956	16.433	41.547
ATOM	3291	O	PHE	328	19.935	16.596	40.880
ATOM	3292	N	LEU	329	21.270	15.262	42.130
ATOM	3293	HN	LEU	329	22.106	15.206	42.730
ATOM	3294	CA	LEU	329	20.470	14.096	41.933
ATOM	3295	HA	LEU	329	20.416	13.895	40.863
ATOM	3296	CB	LEU	329	21.059	12.859	42.644
ATOM	3297	HB1	LEU	329	21.110	13.079	43.711
ATOM	3298	HB2	LEU	329	22.053	12.679	42.234
ATOM	3299	CG	LEU	329	20.262	11.543	42.491
ATOM	3300	HG	LEU	329	20.813	10.667	42.832
ATOM	3301	CD2	LEU	329	20.060	11.202	41.000
ATOM	3302	HD2	LEU	329	19.497	10.273	40.912
ATOM	3303	HD2	LEU	329	19.510	12.008	40.514
ATOM	3304	HD2	LEU	329	21.031	11.085	40.519
ATOM	3305	CD1	LEU	329	18.949	11.540	43.283
ATOM	3306	HD1	LEU	329	18.436	10.590	43.134
ATOM	3307	HD1	LEU	329	19.164	11.674	44.343
ATOM	3308	HD1	LEU	329	18.313	12.354	42.937
ATOM	3309	C	LEU	329	19.112	14.364	42.488
ATOM	3310	O	LEU	329	18.107	14.056	41.848
ATOM	3311	N	LEU	330	19.035	14.962	43.688
ATOM	3312	HN	LEU	330	19.874	15.282	44.193
ATOM	3313	CA	LEU	330	17.722	15.129	44.223
ATOM	3314	HA	LEU	330	17.010	14.721	43.506
ATOM	3315	CB	LEU	330	17.543	14.422	45.576
ATOM	3316	HB1	LEU	330	17.997	15.041	46.349
ATOM	3317	HB2	LEU	330	18.036	13.451	45.523
ATOM	3318	CG	LEU	330	16.072	14.181	45.970
ATOM	3319	HG	LEU	330	15.976	13.716	46.951
ATOM	3320	CD2	LEU	330	15.436	13.109	45.072
ATOM	3321	HD2	LEU	330	14.398	12.955	45.368
ATOM	3322	HD2	LEU	330	15.472	13.437	44.033
ATOM	3323	HD2	LEU	330	15.985	12.174	45.177
ATOM	3324	CD1	LEU	330	15.262	15.482	46.026
ATOM	3325	HD1	LEU	330	14.233	15.258	46.308
ATOM	3326	HD1	LEU	330	15.703	16.153	46.763
ATOM	3327	HD1	LEU	330	15.274	15.960	45.047
ATOM	3328	C	LEU	330	17.487	16.592	44.431
ATOM	3329	O	LEU	330	17.444	17.077	45.562
ATOM	3330	N	ASN	331	17.328	17.341	43.328
ATOM	3331	HN	ASN	331	17.407	16.901	42.400
ATOM	3332	CA	ASN	331	17.051	18.742	43.424
ATOM	3333	HA	ASN	331	17.837	19.170	44.047
ATOM	3334	CB	ASN	331	16.976	19.424	42.048
ATOM	3335	HB1	ASN	331	16.171	18.958	41.480
ATOM	3336	HB2	ASN	331	17.933	19.284	41.544
ATOM	3337	CG	ASN	331	16.694	20.904	42.264
ATOM	3338	OD1	ASN	331	16.194	21.591	41.374
ATOM	3339	ND2	ASN	331	17.027	21.411	43.480
ATOM	3340	HD2	ASN	331	17.444	20.799	44.197
ATOM	3341	HD2	ASN	331	16.863	22.407	43.685
ATOM	3342	C	ASN	331	15.703	18.864	44.050
ATOM	3343	O	ASN	331	15.436	19.785	44.821

ATOM	3344	N	LYS	332	14.823	17.903	43.713
ATOM	3345	HN	LYS	332	15.153	17.154	43.086
ATOM	3346	CA	LYS	332	13.462	17.843	44.159
ATOM	3347	HA	LYS	332	12.928	18.738	43.841
ATOM	3348	CB	LYS	332	12.715	16.655	43.515
ATOM	3349	HB1	LYS	332	12.740	16.788	42.433
ATOM	3350	HB2	LYS	332	11.689	16.662	43.883
ATOM	3351	CG	LYS	332	13.296	15.273	43.816
ATOM	3352	HG1	LYS	332	13.499	15.128	44.877
ATOM	3353	HG2	LYS	332	14.239	15.095	43.298
ATOM	3354	CD	LYS	332	12.355	14.138	43.399
ATOM	3355	HD1	LYS	332	12.076	14.291	42.357
ATOM	3356	HD2	LYS	332	11.475	14.170	44.042
ATOM	3357	CE	LYS	332	12.963	12.738	43.515
ATOM	3358	HE1	LYS	332	13.258	12.543	44.546
ATOM	3359	HE2	LYS	332	13.841	12.657	42.875
ATOM	3360	NZ	LYS	332	11.972	11.719	43.099
ATOM	3361	HZ1	LYS	332	12.389	10.781	43.180
ATOM	3362	HZ2	LYS	332	11.142	11.779	43.706
ATOM	3363	HZ3	LYS	332	11.695	11.888	42.122
ATOM	3364	C	LYS	332	13.419	17.754	45.662
ATOM	3365	O	LYS	332	14.399	18.071	46.332
ATOM	3366	N	PRO	333	12.345	17.329	46.275
ATOM	3367	CA	PRO	333	12.372	17.351	47.704
ATOM	3368	HA	PRO	333	12.569	18.375	48.023
ATOM	3369	CD	PRO	333	10.990	17.562	45.801
ATOM	3370	HD1	PRO	333	10.839	17.134	44.810
ATOM	3371	HD2	PRO	333	10.772	18.628	45.737
ATOM	3372	CB	PRO	333	10.943	17.070	48.173
ATOM	3373	HB1	PRO	333	10.656	17.963	48.728
ATOM	3374	HB2	PRO	333	11.028	16.175	48.789
ATOM	3375	CG	PRO	333	10.141	16.860	46.870
ATOM	3376	HG1	PRO	333	9.148	17.302	46.948
ATOM	3377	HG2	PRO	333	10.021	15.798	46.654
ATOM	3378	C	PRO	333	13.404	16.485	48.328
ATOM	3379	O	PRO	333	13.222	15.270	48.380
ATOM	3380	N	THR	334	14.503	17.100	48.802
ATOM	3381	HN	THR	334	14.657	18.101	48.614
ATOM	3382	CA	THR	334	15.454	16.361	49.568
ATOM	3383	HA	THR	334	14.917	15.955	50.425
ATOM	3384	CB	THR	334	16.184	15.293	48.819
ATOM	3385	HB	THR	334	15.468	14.836	48.137
ATOM	3386	OG1	THR	334	16.744	14.358	49.730
ATOM	3387	HG1	THR	334	16.396	14.553	50.680
ATOM	3388	CG2	THR	334	17.332	15.979	48.066
ATOM	3389	HG2	THR	334	17.895	15.234	47.503
ATOM	3390	HG2	THR	334	16.925	16.721	47.379
ATOM	3391	HG2	THR	334	17.994	16.471	48.779
ATOM	3392	C	THR	334	16.513	17.324	49.973
ATOM	3393	O	THR	334	17.386	16.980	50.767
ATOM	3394	N	LYS	335	16.445	18.569	49.459
ATOM	3395	HN	LYS	335	15.670	18.833	48.834
ATOM	3396	CA	LYS	335	17.463	19.521	49.793
ATOM	3397	HA	LYS	335	18.411	19.126	49.429
ATOM	3398	CB	LYS	335	17.278	20.909	49.153
ATOM	3399	HB1	LYS	335	16.280	21.324	49.291
ATOM	3400	HB2	LYS	335	17.441	20.918	48.075
ATOM	3401	CG	LYS	335	18.229	21.970	49.706
ATOM	3402	HG1	LYS	335	18.105	22.009	50.788
ATOM	3403	HG2	LYS	335	17.971	22.928	49.255
ATOM	3404	CD	LYS	335	19.705	21.709	49.420
ATOM	3405	HD1	LYS	335	19.938	21.661	48.356
ATOM	3406	HD2	LYS	335	20.067	20.769	49.837
ATOM	3407	CE	LYS	335	20.633	22.785	49.987
ATOM	3408	HE1	LYS	335	20.509	22.855	51.068
ATOM	3409	HE2	LYS	335	20.399	23.753	49.542
ATOM	3410	NZ	LYS	335	22.043	22.448	49.688
ATOM	3411	HZ1	LYS	335	22.660	23.178	50.073

	ATOM	3412	HZ2	LYS	335	22.277	21.541	50.114
	ATOM	3413	HZ3	LYS	335	22.174	22.392	48.668
	ATOM	3414	C	LYS	335	17.466	19.668	51.276
	ATOM	3415	O	LYS	335	16.479	20.090	51.878
5	ATOM	3416	N	ILE	336	18.609	19.311	51.894
	ATOM	3417	HN	ILE	336	19.416	19.017	51.326
	ATOM	3418	CA	ILE	336	18.728	19.330	53.318
	ATOM	3419	HA	ILE	336	18.033	18.591	53.715
	ATOM	3420	CB	ILE	336	20.119	19.029	53.790
10	ATOM	3421	HB	ILE	336	20.798	19.724	53.296
	ATOM	3422	CG2	ILE	336	20.151	19.218	55.317
	ATOM	3423	HG2	ILE	336	21.153	19.005	55.689
	ATOM	3424	HG2	ILE	336	19.884	20.246	55.562
	ATOM	3425	HG2	ILE	336	19.439	18.537	55.783
15	ATOM	3426	CG1	ILE	336	20.547	17.623	53.337
	ATOM	3427	HG1	ILE	336	21.559	17.358	53.640
	ATOM	3428	HG1	ILE	336	20.530	17.492	52.255
	ATOM	3429	CD1	ILE	336	19.659	16.509	53.889
	ATOM	3430	HD1	ILE	336	20.018	15.545	53.528
20	ATOM	3431	HD1	ILE	336	19.691	16.524	54.978
	ATOM	3432	HD1	ILE	336	18.633	16.662	53.554
	ATOM	3433	C	ILE	336	18.382	20.700	53.777
	ATOM	3434	O	ILE	336	17.575	20.864	54.690
	ATOM	3435	N	LEU	337	18.982	21.729	53.151
25	ATOM	3436	HN	LEU	337	19.674	21.566	52.405
	ATOM	3437	CA	LEU	337	18.631	23.055	53.553
	ATOM	3438	HA	LEU	337	18.867	23.081	54.617
	ATOM	3439	CB	LEU	337	19.395	24.134	52.758
	ATOM	3440	HB1	LEU	337	19.028	24.117	51.732
30	ATOM	3441	HB2	LEU	337	20.457	23.889	52.796
	ATOM	3442	CG	LEU	337	19.243	25.585	53.272
	ATOM	3443	HG	LEU	337	19.605	25.670	54.297
	ATOM	3444	CD2	LEU	337	17.779	26.024	53.416
	ATOM	3445	HD2	LEU	337	17.741	27.051	53.780
35	ATOM	3446	HD2	LEU	337	17.284	25.965	52.446
	ATOM	3447	HD2	LEU	337	17.270	25.369	54.123
	ATOM	3448	CD1	LEU	337	20.047	26.557	52.396
	ATOM	3449	HD1	LEU	337	19.927	27.573	52.775
	ATOM	3450	HD1	LEU	337	21.102	26.283	52.422
40	ATOM	3451	HD1	LEU	337	19.684	26.508	51.370
	ATOM	3452	C	LEU	337	17.177	23.154	53.246
	ATOM	3453	O	LEU	337	16.363	23.423	54.127
	ATOM	3454	N	SER	338	16.815	22.904	51.972
	ATOM	3455	HN	SER	338	17.540	22.720	51.263
45	ATOM	3456	CA	SER	338	15.436	22.893	51.593
	ATOM	3457	HA	SER	338	14.985	21.977	51.975
	ATOM	3458	CB	SER	338	14.632	24.099	52.112
	ATOM	3459	HB1	SER	338	15.054	25.026	51.722
	ATOM	3460	HB2	SER	338	14.663	24.129	53.201
50	ATOM	3461	OG	SER	338	13.279	24.000	51.694
	ATOM	3462	HG	SER	338	12.822	24.919	51.786
	ATOM	3463	C	SER	338	15.360	22.935	50.106
	ATOM	3464	O	SER	338	16.069	23.692	49.445
	ATOM	3465	N	PRO	339	14.516	22.103	49.568
55	ATOM	3466	CA	PRO	339	14.255	22.163	48.161
	ATOM	3467	HA	PRO	339	15.088	22.609	47.617
	ATOM	3468	CD	PRO	339	14.402	20.747	50.076
	ATOM	3469	HD1	PRO	339	13.856	20.842	51.015
	ATOM	3470	HD2	PRO	339	15.429	20.405	50.202
60	ATOM	3471	CB	PRO	339	13.990	20.730	47.702
	ATOM	3472	HB1	PRO	339	14.931	20.414	47.251
	ATOM	3473	HB2	PRO	339	13.166	20.822	46.996
	ATOM	3474	CG	PRO	339	13.630	19.980	48.993
	ATOM	3475	HG1	PRO	339	13.939	18.936	48.938
65	ATOM	3476	HG2	PRO	339	12.555	20.001	49.171
	ATOM	3477	C	PRO	339	13.035	23.010	48.130
	ATOM	3478	O	PRO	339	12.498	23.283	49.203
	ATOM	3479	N	GLU	340	12.566	23.426	46.943

ATOM	3480	HN	GLU	340	13.039	23.165	46.066
ATOM	3481	CA	GLU	340	11.393	24.242	46.929
ATOM	3482	HA	GLU	340	11.639	25.128	47.513
ATOM	3483	CB	GLU	340	10.903	24.629	45.525
ATOM	3484	HB1	GLU	340	10.465	23.789	44.985
ATOM	3485	HB2	GLU	340	11.702	25.011	44.890
ATOM	3486	CG	GLU	340	9.828	25.719	45.553
ATOM	3487	HG1	GLU	340	10.290	26.661	45.847
ATOM	3488	HG2	GLU	340	9.060	25.437	46.273
ATOM	3489	CD	GLU	340	9.220	25.846	44.163
ATOM	3490	OE1	GLU	340	9.038	24.792	43.499
ATOM	3491	OE2	GLU	340	8.910	26.997	43.756
ATOM	3493	C	GLU	340	10.319	23.421	47.551
ATOM	3494	O	GLU	340	9.411	23.946	48.192
ATOM	3495	N	TYR	341	10.412	22.087	47.387
ATOM	3496	HN	TYR	341	11.209	21.680	46.877
ATOM	3497	CA	TYR	341	9.395	21.245	47.929
ATOM	3498	HA	TYR	341	8.461	21.552	47.458
ATOM	3499	CB	TYR	341	9.632	19.753	47.675
ATOM	3500	HB1	TYR	341	10.303	19.407	48.461
ATOM	3501	HB2	TYR	341	10.081	19.674	46.685
ATOM	3502	CG	TYR	341	8.300	19.094	47.743
ATOM	3503	CD1	TYR	341	7.518	19.074	46.613
ATOM	3504	HD1	TYR	341	7.882	19.541	45.698
ATOM	3505	CD2	TYR	341	7.831	18.510	48.895
ATOM	3506	HD2	TYR	341	8.438	18.525	49.800
ATOM	3507	CE1	TYR	341	6.284	18.473	46.621
ATOM	3508	HE1	TYR	341	5.679	18.453	45.714
ATOM	3509	CE2	TYR	341	6.594	17.906	48.907
ATOM	3510	HE2	TYR	341	6.230	17.433	49.819
ATOM	3511	CZ	TYR	341	5.816	17.898	47.774
ATOM	3512	OH	TYR	341	4.549	17.279	47.794
ATOM	3513	HH	TYR	341	3.827	17.980	48.016
ATOM	3514	C	TYR	341	9.395	21.484	49.404
ATOM	3515	O	TYR	341	10.318	22.088	49.946
ATOM	3516	N	CYS	342	8.345	21.014	50.097
ATOM	3517	HN	CYS	342	7.623	20.457	49.618
ATOM	3518	CA	CYS	342	8.225	21.281	51.499
ATOM	3519	HA	CYS	342	8.441	22.333	51.687
ATOM	3520	CB	CYS	342	6.811	20.969	52.020
ATOM	3521	HB1	CYS	342	6.520	19.927	51.884
ATOM	3522	HB2	CYS	342	6.031	21.552	51.529
ATOM	3523	SG	CYS	342	6.610	21.296	53.793
ATOM	3524	HG	CYS	342	7.043	22.533	54.072
ATOM	3525	C	CYS	342	9.196	20.428	52.255
ATOM	3526	O	CYS	342	8.801	19.459	52.902
ATOM	3527	N	TRP	343	10.498	20.774	52.202
ATOM	3528	HN	TRP	343	10.795	21.575	51.627
ATOM	3529	CA	TRP	343	11.470	20.028	52.947
ATOM	3530	HA	TRP	343	11.348	18.981	52.669
ATOM	3531	CB	TRP	343	12.913	20.484	52.698
ATOM	3532	HB1	TRP	343	13.091	21.526	52.963
ATOM	3533	HB2	TRP	343	13.223	20.397	51.657
ATOM	3534	CG	TRP	343	13.937	19.696	53.482
ATOM	3535	CD2	TRP	343	14.489	20.117	54.739
ATOM	3536	CD1	TRP	343	14.520	18.497	53.186
ATOM	3537	HD1	TRP	343	14.321	17.909	52.290
ATOM	3538	NE1	TRP	343	15.394	18.141	54.186
ATOM	3539	HE1	TRP	343	15.959	17.281	54.213
ATOM	3540	CE2	TRP	343	15.387	19.130	55.147
ATOM	3541	CE3	TRP	343	14.264	21.234	55.492
ATOM	3542	HE3	TRP	343	13.561	22.002	55.172
ATOM	3543	CZ2	TRP	343	16.075	19.245	56.322
ATOM	3544	HZ2	TRP	343	16.774	18.475	56.647
ATOM	3545	CZ3	TRP	343	14.964	21.348	56.673
ATOM	3546	HZ3	TRP	343	14.814	22.228	57.300
ATOM	3547	CH2	TRP	343	15.851	20.373	57.080
ATOM	3548	HH2	TRP	343	16.385	20.497	58.022

ATOM	3549	C	TRP	343	11.180	20.256	54.394
ATOM	3550	O	TRP	343	11.151	19.320	55.189
ATOM	3551	N	ASP	344	10.955	21.527	54.770
ATOM	3552	HN	ASP	344	11.001	22.283	54.072
ATOM	3553	CA	ASP	344	10.650	21.836	56.137
ATOM	3554	HA	ASP	344	10.573	20.877	56.651
ATOM	3555	CB	ASP	344	11.687	22.748	56.812
ATOM	3556	HB1	ASP	344	12.658	22.257	56.752
ATOM	3557	HB2	ASP	344	11.388	22.890	57.850
ATOM	3558	CG	ASP	344	11.704	24.075	56.066
ATOM	3559	OD1	ASP	344	11.690	24.046	54.807
ATOM	3560	OD2	ASP	344	11.738	25.136	56.745
ATOM	3561	C	ASP	344	9.360	22.580	56.111
ATOM	3562	O	ASP	344	8.754	22.715	55.051
ATOM	3563	N	TYR	345	8.913	23.047	57.296
ATOM	3564	HN	TYR	345	9.471	22.833	58.134
ATOM	3565	CA	TYR	345	7.713	23.820	57.473
ATOM	3566	HA	TYR	345	7.873	24.541	58.275
ATOM	3567	CB	TYR	345	7.279	24.664	56.257
ATOM	3568	HB1	TYR	345	6.334	25.147	56.507
ATOM	3569	HB2	TYR	345	7.163	23.991	55.408
ATOM	3570	CG	TYR	345	8.344	25.674	55.999
ATOM	3571	CD1	TYR	345	8.405	26.833	56.739
ATOM	3572	HD1	TYR	345	7.668	27.013	57.521
ATOM	3573	CD2	TYR	345	9.279	25.464	55.012
ATOM	3574	HD2	TYR	345	9.240	24.552	54.417
ATOM	3575	CE1	TYR	345	9.387	27.766	56.499
ATOM	3576	HE1	TYR	345	9.426	28.680	57.092
ATOM	3577	CE2	TYR	345	10.263	26.393	54.769
ATOM	3578	HE2	TYR	345	11.000	26.215	53.985
ATOM	3579	CZ	TYR	345	10.318	27.546	55.513
ATOM	3580	OH	TYR	345	11.326	28.500	55.264
ATOM	3581	HH	TYR	345	12.183	28.235	55.769
ATOM	3582	C	TYR	345	6.593	22.901	57.828
ATOM	3583	O	TYR	345	6.663	22.172	58.815
ATOM	3584	N	HIS	346	5.517	22.921	57.018
ATOM	3585	HN	HIS	346	5.531	23.508	56.172
ATOM	3586	CA	HIS	346	4.352	22.138	57.312
ATOM	3587	HA	HIS	346	4.231	22.053	58.392
ATOM	3588	ND1	HIS	346	2.100	24.270	58.548
ATOM	3589	HD1	HIS	346	1.748	23.531	59.174
ATOM	3590	CG	HIS	346	2.747	24.090	57.346
ATOM	3591	NE2	HIS	346	2.559	26.299	57.763
ATOM	3592	HE2	HIS	346	2.625	27.323	57.671
ATOM	3593	CD2	HIS	346	3.020	25.339	56.880
ATOM	3594	HD2	HIS	346	3.532	25.553	55.942
ATOM	3595	CE1	HIS	346	2.013	25.609	58.748
ATOM	3596	HE1	HIS	346	1.548	26.064	59.623
ATOM	3597	CB	HIS	346	3.057	22.749	56.750
ATOM	3598	HB1	HIS	346	2.184	22.124	56.938
ATOM	3599	HB2	HIS	346	3.098	22.898	55.671
ATOM	3600	C	HIS	346	4.501	20.774	56.722
ATOM	3601	O	HIS	346	5.584	20.370	56.303
ATOM	3602	N	ILE	347	3.386	20.016	56.706
ATOM	3603	HN	ILE	347	2.511	20.405	57.086
ATOM	3604	CA	ILE	347	3.382	18.685	56.175
ATOM	3605	HA	ILE	347	4.426	18.419	56.014
ATOM	3606	CB	ILE	347	2.720	17.696	57.097
ATOM	3607	HB	ILE	347	1.703	18.029	57.308
ATOM	3608	CG2	ILE	347	2.685	16.317	56.415
ATOM	3609	HG2	ILE	347	2.206	15.596	57.078
ATOM	3610	HG2	ILE	347	2.121	16.385	55.485
ATOM	3611	HG2	ILE	347	3.703	15.992	56.200
ATOM	3612	CG1	ILE	347	3.452	17.675	58.449
ATOM	3613	HG1	ILE	347	3.633	18.667	58.862
ATOM	3614	HG1	ILE	347	4.433	17.202	58.406
ATOM	3615	CD1	ILE	347	2.696	16.922	59.541
ATOM	3616	HD1	ILE	347	3.271	16.948	60.467

ATOM	3617	HD1	ILE	347	1.726	17.393	59.703
ATOM	3618	HD1	ILE	347	2.549	15.886	59.234
ATOM	3619	C	ILE	347	2.603	18.747	54.899
ATOM	3620	O	ILE	347	1.826	19.676	54.687
ATOM	3621	N	GLY	348	2.806	17.764	53.999
ATOM	3622	HN	GLY	348	3.450	16.991	54.220
ATOM	3623	CA	GLY	348	2.130	17.791	52.735
ATOM	3624	HA1	GLY	348	2.777	17.356	51.974
ATOM	3625	HA2	GLY	348	1.898	18.824	52.476
ATOM	3626	C	GLY	348	0.865	16.999	52.839
ATOM	3627	O	GLY	348	0.819	15.955	53.488
ATOM	3628	N	LEU	349	-0.199	17.489	52.169
ATOM	3629	HN	LEU	349	-0.093	18.365	51.638
ATOM	3630	CA	LEU	349	-1.474	16.829	52.172
ATOM	3631	HA	LEU	349	-1.474	16.133	53.011
ATOM	3632	CB	LEU	349	-2.666	17.793	52.297
ATOM	3633	HB1	LEU	349	-3.634	17.298	52.226
ATOM	3634	HB2	LEU	349	-2.683	18.565	51.527
ATOM	3635	CG	LEU	349	-2.701	18.557	53.634
ATOM	3636	HG	LEU	349	-3.510	19.288	53.652
ATOM	3637	CD2	LEU	349	-1.462	19.452	53.800
ATOM	3638	HD2	LEU	349	-1.518	19.977	54.754
ATOM	3639	HD2	LEU	349	-0.563	18.836	53.777
ATOM	3640	HD2	LEU	349	-1.425	20.178	52.988
ATOM	3641	CD1	LEU	349	-2.913	17.601	54.819
ATOM	3642	HD1	LEU	349	-2.933	18.172	55.748
ATOM	3643	HD1	LEU	349	-3.860	17.074	54.697
ATOM	3644	HD1	LEU	349	-2.098	16.879	54.854
ATOM	3645	C	LEU	349	-1.606	16.118	50.863
ATOM	3646	O	LEU	349	-1.295	16.653	49.799
ATOM	3647	N	PRO	350	-2.044	14.895	50.948
ATOM	3648	CA	PRO	350	-2.150	14.088	49.763
ATOM	3649	HA	PRO	350	-1.272	14.281	49.147
ATOM	3650	CD	PRO	350	-1.680	14.100	52.112
ATOM	3651	HD1	PRO	350	-2.555	14.110	52.762
ATOM	3652	HD2	PRO	350	-0.817	14.601	52.553
ATOM	3653	CB	PRO	350	-2.095	12.634	50.233
ATOM	3654	HB1	PRO	350	-1.550	12.120	49.442
ATOM	3655	HB2	PRO	350	-3.142	12.343	50.318
ATOM	3656	CG	PRO	350	-1.349	12.702	51.573
ATOM	3657	HG1	PRO	350	-0.303	12.561	51.301
ATOM	3658	HG2	PRO	350	-1.776	11.885	52.154
ATOM	3659	C	PRO	350	-3.349	14.333	48.904
ATOM	3660	O	PRO	350	-4.389	14.753	49.409
ATOM	3661	N	ALA	351	-3.196	14.076	47.590
ATOM	3662	HN	ALA	351	-2.249	13.861	47.246
ATOM	3663	CA	ALA	351	-4.271	14.084	46.642
ATOM	3664	HA	ALA	351	-5.229	14.262	47.131
ATOM	3665	CB	ALA	351	-4.081	15.093	45.497
ATOM	3666	HB1	ALA	351	-4.934	15.041	44.821
ATOM	3667	HB2	ALA	351	-4.005	16.099	45.909
ATOM	3668	HB3	ALA	351	-3.169	14.854	44.950
ATOM	3669	C	ALA	351	-4.186	12.713	46.052
ATOM	3670	O	ALA	351	-3.225	12.399	45.352
ATOM	3671	N	ASP	352	-5.192	11.857	46.309
ATOM	3672	HN	ASP	352	-6.044	12.188	46.784
ATOM	3673	CA	ASP	352	-5.073	10.481	45.917
ATOM	3674	HA	ASP	352	-4.059	10.115	46.077
ATOM	3675	CB	ASP	352	-6.015	9.561	46.717
ATOM	3676	HB1	ASP	352	-7.046	9.710	46.396
ATOM	3677	HB2	ASP	352	-5.942	9.784	47.781
ATOM	3678	CG	ASP	352	-5.636	8.100	46.493
ATOM	3679	OD1	ASP	352	-5.393	7.704	45.322
ATOM	3680	OD2	ASP	352	-5.597	7.354	47.506
ATOM	3681	C	ASP	352	-5.401	10.306	44.469
ATOM	3682	O	ASP	352	-6.490	9.847	44.128
ATOM	3683	N	ILE	353	-4.451	10.655	43.580
ATOM	3684	HN	ILE	353	-3.585	11.100	43.918

```
ATOM   3685  CA  ILE   353      -4.614  10.421  42.174
ATOM   3686  HA  ILE   353      -5.130   9.465  42.076
ATOM   3687  CB  ILE   353      -5.385  11.489  41.444
ATOM   3688  HB  ILE   353      -5.369  11.263  40.378
ATOM   3689  CG2 ILE   353      -6.831  11.495  41.967
ATOM   3690  HG2 ILE   353      -7.403  12.264  41.447
ATOM   3691  HG2 ILE   353      -7.287  10.521  41.787
ATOM   3692  HG2 ILE   353      -6.831  11.703  43.036
ATOM   3693  CG1 ILE   353      -4.682  12.852  41.552
ATOM   3694  HG1 ILE   353      -5.226  13.569  40.939
ATOM   3695  HG1 ILE   353      -3.659  12.739  41.192
ATOM   3696  CD1 ILE   353      -4.617  13.407  42.974
ATOM   3697  HD1 ILE   353      -4.106  14.370  42.966
ATOM   3698  HD1 ILE   353      -5.628  13.537  43.361
ATOM   3699  HD1 ILE   353      -4.071  12.712  43.612
ATOM   3700  C   ILE   353      -3.240  10.386  41.586
ATOM   3701  O   ILE   353      -2.372  11.154  41.993
ATOM   3702  N   LYS   354      -2.986   9.477  40.623
ATOM   3703  HN  LYS   354      -3.706   8.806  40.319
ATOM   3704  CA  LYS   354      -1.676   9.479  40.039
ATOM   3705  HA  LYS   354      -1.013   9.932  40.777
ATOM   3706  CB  LYS   354      -1.200   8.073  39.637
ATOM   3707  HB1 LYS   354      -0.230   8.069  39.140
ATOM   3708  HB2 LYS   354      -1.877   7.567  38.949
ATOM   3709  CG  LYS   354      -1.047   7.120  40.824
ATOM   3710  HG1 LYS   354      -0.453   7.527  41.643
ATOM   3711  HG2 LYS   354      -0.563   6.176  40.572
ATOM   3712  CD  LYS   354      -2.375   6.717  41.469
ATOM   3713  HD1 LYS   354      -3.055   6.210  40.784
ATOM   3714  HD2 LYS   354      -2.943   7.561  41.860
ATOM   3715  CE  LYS   354      -2.215   5.761  42.652
ATOM   3716  HE1 LYS   354      -1.608   6.227  43.427
ATOM   3717  HE2 LYS   354      -1.729   4.842  42.324
ATOM   3718  NZ  LYS   354      -3.543   5.428  43.215
ATOM   3719  HZ1 LYS   354      -3.427   4.784  44.011
ATOM   3720  HZ2 LYS   354      -4.006   6.290  43.536
ATOM   3721  HZ3 LYS   354      -4.121   4.978  42.491
ATOM   3722  C   LYS   354      -1.776  10.287  38.791
ATOM   3723  O   LYS   354      -1.149   9.986  37.778
ATOM   3724  N   LEU   355      -2.588  11.352  38.843
ATOM   3725  HN  LEU   355      -3.084  11.560  39.721
ATOM   3726  CA  LEU   355      -2.787  12.208  37.714
ATOM   3727  HA  LEU   355      -2.937  11.591  36.828
ATOM   3728  CB  LEU   355      -3.989  13.145  37.908
ATOM   3729  HB1 LEU   355      -4.228  13.731  37.021
ATOM   3730  HB2 LEU   355      -3.845  13.875  38.704
ATOM   3731  CG  LEU   355      -5.290  12.404  38.267
ATOM   3732  HG  LEU   355      -5.209  11.908  39.234
ATOM   3733  CD2 LEU   355      -5.537  11.204  37.343
ATOM   3734  HD2 LEU   355      -6.464  10.708  37.629
ATOM   3735  HD2 LEU   355      -5.613  11.548  36.312
ATOM   3736  HD2 LEU   355      -4.708  10.501  37.430
ATOM   3737  CD1 LEU   355      -6.482  13.372  38.340
ATOM   3738  HD1 LEU   355      -7.385  12.818  38.596
ATOM   3739  HD1 LEU   355      -6.291  14.127  39.103
ATOM   3740  HD1 LEU   355      -6.615  13.858  37.374
ATOM   3741  C   LEU   355      -1.577  13.067  37.545
ATOM   3742  O   LEU   355      -1.167  13.390  36.432
ATOM   3743  N   VAL   356      -0.974  13.447  38.680
ATOM   3744  HN  VAL   356      -1.281  13.031  39.571
ATOM   3745  CA  VAL   356       0.081  14.411  38.695
ATOM   3746  HA  VAL   356      -0.239  15.400  38.370
ATOM   3747  CB  VAL   356       0.613  14.654  40.076
ATOM   3748  HB  VAL   356      -0.188  15.056  40.696
ATOM   3749  CG1 VAL   356       1.113  13.323  40.656
ATOM   3750  HG1 VAL   356       1.503  13.488  41.661
ATOM   3751  HG1 VAL   356       0.289  12.612  40.699
ATOM   3752  HG1 VAL   356       1.905  12.924  40.021
```

ATOM	3753	CG2	VAL	356	1.686	15.754	39.997
ATOM	3754	HG2	VAL	356	2.085	15.945	40.993
ATOM	3755	HG2	VAL	356	2.492	15.429	39.340
ATOM	3756	HG2	VAL	356	1.242	16.668	39.603
ATOM	3757	C	VAL	356	1.224	14.042	37.801
ATOM	3758	O	VAL	356	1.563	14.814	36.907
ATOM	3759	N	LYS	357	1.857	12.864	37.971
ATOM	3760	HN	LYS	357	1.538	12.139	38.628
ATOM	3761	CA	LYS	357	3.021	12.723	37.145
ATOM	3762	HA	LYS	357	3.075	13.488	36.370
ATOM	3763	CB	LYS	357	4.366	12.769	37.900
ATOM	3764	HB1	LYS	357	5.164	12.753	37.158
ATOM	3765	HB2	LYS	357	4.412	11.894	38.548
ATOM	3766	CG	LYS	357	4.616	13.991	38.790
ATOM	3767	HG1	LYS	357	4.238	14.919	38.361
ATOM	3768	HG2	LYS	357	5.673	14.170	38.986
ATOM	3769	CD	LYS	357	3.959	13.879	40.166
ATOM	3770	HD1	LYS	357	4.246	12.924	40.606
ATOM	3771	HD2	LYS	357	2.878	13.932	40.033
ATOM	3772	CE	LYS	357	4.358	14.980	41.150
ATOM	3773	HE1	LYS	357	4.076	15.953	40.750
ATOM	3774	HE2	LYS	357	5.435	14.958	41.312
ATOM	3775	NZ	LYS	357	3.668	14.770	42.444
ATOM	3776	HZ1	LYS	357	3.940	15.513	43.103
ATOM	3777	HZ2	LYS	357	2.649	14.796	42.299
ATOM	3778	HZ3	LYS	357	3.936	13.854	42.831
ATOM	3779	C	LYS	357	3.062	11.409	36.443
ATOM	3780	O	LYS	357	2.441	10.425	36.844
ATOM	3781	N	MET	358	3.820	11.423	35.329
ATOM	3782	HN	MET	358	4.173	12.343	35.030
ATOM	3783	CA	MET	358	4.194	10.306	34.514
ATOM	3784	HA	MET	358	4.098	9.364	35.054
ATOM	3785	CB	MET	358	3.394	10.245	33.203
ATOM	3786	HB1	MET	358	3.750	11.041	32.550
ATOM	3787	HB2	MET	358	2.339	10.383	33.441
ATOM	3788	CG	MET	358	3.524	8.931	32.439
ATOM	3789	HG1	MET	358	3.163	8.127	33.081
ATOM	3790	HG2	MET	358	4.576	8.785	32.191
ATOM	3791	SD	MET	358	2.583	8.851	30.885
ATOM	3792	CE	MET	358	3.706	9.922	29.944
ATOM	3793	HE1	MET	358	3.335	10.032	28.925
ATOM	3794	HE2	MET	358	3.758	10.901	30.419
ATOM	3795	HE3	MET	358	4.700	9.476	29.922
ATOM	3796	C	MET	358	5.620	10.646	34.193
ATOM	3797	O	MET	358	5.921	11.821	33.992
ATOM	3798	N	SER	359	6.563	9.678	34.147
ATOM	3799	HN	SER	359	6.347	8.674	34.227
ATOM	3800	CA	SER	359	7.899	10.188	33.975
ATOM	3801	HA	SER	359	7.932	11.039	33.296
ATOM	3802	CB	SER	359	8.435	10.752	35.314
ATOM	3803	HB1	SER	359	8.438	10.019	36.121
ATOM	3804	HB2	SER	359	7.855	11.594	35.691
ATOM	3805	OG	SER	359	9.770	11.223	35.231
ATOM	3806	HG	SER	359	10.404	10.542	35.672
ATOM	3807	C	SER	359	8.838	9.150	33.409
ATOM	3808	O	SER	359	8.455	8.052	33.024
ATOM	3809	N	TRP	360	10.120	9.515	33.241
ATOM	3810	HN	TRP	360	10.396	10.491	33.419
ATOM	3811	CA	TRP	360	11.110	8.569	32.818
ATOM	3812	HA	TRP	360	10.756	7.591	33.145
ATOM	3813	CB	TRP	360	11.354	8.542	31.297
ATOM	3814	HB1	TRP	360	12.306	8.044	31.111
ATOM	3815	HB2	TRP	360	11.383	9.570	30.936
ATOM	3816	CG	TRP	360	10.290	7.809	30.512
ATOM	3817	CD2	TRP	360	9.025	8.364	30.117
ATOM	3818	CD1	TRP	360	10.307	6.524	30.054
ATOM	3819	HD1	TRP	360	11.130	5.823	30.191
ATOM	3820	NE1	TRP	360	9.135	6.244	29.396

	ATOM	3821	HE1	TRP	360	8.893	5.346	28.952
	ATOM	3822	CE2	TRP	360	8.336	7.367	29.428
	ATOM	3823	CE3	TRP	360	8.482	9.600	30.315
	ATOM	3824	HE3	TRP	360	9.021	10.378	30.857
5	ATOM	3825	CZ2	TRP	360	7.087	7.591	28.924
	ATOM	3826	HZ2	TRP	360	6.545	6.813	28.386
	ATOM	3827	CZ3	TRP	360	7.223	9.824	29.802
	ATOM	3828	HZ3	TRP	360	6.758	10.800	29.938
	ATOM	3829	CH2	TRP	360	6.538	8.840	29.121
10	ATOM	3830	HH2	TRP	360	5.544	9.054	28.730
	ATOM	3831	C	TRP	360	12.381	8.970	33.487
	ATOM	3832	O	TRP	360	12.598	10.150	33.753
	ATOM	3833	N	GLN	361	13.264	7.996	33.790
	ATOM	3834	HN	GLN	361	13.084	7.016	33.531
15	ATOM	3835	CA	GLN	361	14.460	8.370	34.486
	ATOM	3836	HA	GLN	361	14.467	9.444	34.669
	ATOM	3837	CB	GLN	361	14.621	7.684	35.851
	ATOM	3838	HB1	GLN	361	14.654	6.597	35.790
	ATOM	3839	HB2	GLN	361	13.811	7.906	36.546
20	ATOM	3840	CG	GLN	361	15.902	8.084	36.587
	ATOM	3841	HG1	GLN	361	15.875	9.162	36.749
	ATOM	3842	HG2	GLN	361	16.750	7.806	35.962
	ATOM	3843	CD	GLN	361	15.935	7.338	37.912
	ATOM	3844	OE1	GLN	361	15.019	6.582	38.234
25	ATOM	3845	NE2	GLN	361	17.017	7.555	38.705
	ATOM	3846	HE2	GLN	361	17.762	8.197	38.396
	ATOM	3847	HE2	GLN	361	17.093	7.079	39.615
	ATOM	3848	C	GLN	361	15.662	8.012	33.670
	ATOM	3849	HC	GLN	361	16.428	8.765	33.483
30	ATOM	3850	O	GLN	361	15.798	6.880	33.208
	ATOM	3851	MN	MET	362	15.622	12.956	35.080

Table 5

Residue number will be set to the conformation's cluster rank.

```
MODEL        9
USER    Run = 9
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       =-2.450 A
USER
USER    Estimated Free Energy of Binding    =   -8.72 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +4.04e-07      [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.73 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.90 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.82 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.520614 19.803704 34.894085
USER    NEWDPF quat0-0.767123 -0.504336 0.396444 20.877983
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-172.23 93.36 -16.11 -9.99 -31.01 0.20 156.88
USER
USER                    Rank         x       y       z       vdW    Elec       q     RMS
ATOM      1  N1   UDP     1      18.167  20.363  33.367    -0.38   -0.11  -0.211  2.450
ATOM      2  C2   UDP     1      18.485  21.574  32.818    -0.84   +0.28  +0.396  2.450
ATOM      3  N3   UDP     1      19.821  21.872  32.732    -0.53   -0.40  -0.440  2.450
ATOM      4  H3   UDP     1      20.069  22.789  32.334    +0.07   +0.53  +0.440  2.450
ATOM      5  C4   UDP     1      20.878  21.052  33.133    -0.75   +0.30  +0.396  2.450
ATOM      6  C5   UDP     1      20.479  19.798  33.691    -0.55   +0.00  +0.000  2.450
ATOM      7  C6   UDP     1      19.174  19.496  33.774    -0.49   +0.00  +0.000  2.450
ATOM      8  O2   UDP     1      17.619  22.362  32.433    -0.35   -0.26  -0.396  2.450
ATOM      9  O4   UDP     1      22.026  21.474  32.994    -0.24   -0.27  -0.396  2.450
ATOM     10  C1'  UDP     1      16.753  19.988  33.503    -0.65   +0.07  +0.324  2.450
ATOM     11  C2'  UDP     1      16.402  18.617  32.920    -0.60   +0.00  +0.113  2.450
ATOM     12  C3'  UDP     1      15.116  18.296  33.717    -0.67   +0.00  +0.113  2.450
ATOM     13  C4'  UDP     1      15.358  18.950  35.076    -0.56   +0.02  +0.113  2.450
ATOM     14  O4'  UDP     1      16.521  19.804  34.894    -0.07   -0.07  -0.227  2.450
ATOM     15  O2'  UDP     1      16.102  18.725  31.548    -0.24   +0.17  -0.537  2.450
ATOM     16  HO2'UDP     1      15.697  17.839  31.214    -0.28   -0.47  +0.424  2.450
ATOM     17  O3'  UDP     1      14.035  18.955  33.051    -0.27   +0.16  -0.537  2.450
ATOM     18  HO3'UDP     1      14.102  18.785  32.037    -0.17   -0.28  +0.424  2.450
ATOM     19  C5'  UDP     1      15.666  17.939  36.181    -0.30   +0.04  +0.113  2.450
ATOM     20  O5'  UDP     1      15.126  18.439  37.390    +0.00   -0.18  -0.368  2.450
ATOM     21  PA   UDP     1      15.642  18.457  38.881    -0.61   +0.45  +1.019  2.450
ATOM     22  O1A  UDP     1      17.132  18.480  38.845    -0.15   -0.08  -0.255  2.450
ATOM     23  O2A  UDP     1      14.933  19.550  39.617    -0.24   -0.09  -0.255  2.450
ATOM     24  O3A  UDP     1      15.133  16.987  39.239    -0.07   -0.23  -0.510  2.450
ATOM     25  PB   UDP     1      15.835  15.723  39.920    -0.72   +0.43  +1.019  2.450
ATOM     26  O1B  UDP     1      15.020  14.448  39.353    -0.03   -0.11  -0.255  2.450
ATOM     27  O2B  UDP     1      15.532  15.971  41.352    -0.68   -0.23  -0.255  2.450
ATOM     28  O3B  UDP     1      17.233  15.484  39.480    -0.12   -0.06  -0.255  2.450
TER
ENDMDL
MODEL       94
USER    Run = 94
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.311 A
USER
```

```
USER    Estimated Free Energy of Binding    =   -8.70 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +4.17e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.71 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.88 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.82 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.394484 19.723058 34.607480
USER    NEWDPF quat00.577475 0.654292 -0.488287 -20.995277
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-101.36 -19.47 179.91 29.29 -15.02 1.94 142.30
USER
USER                    Rank         x       y       z       vdW    Elec       q     RMS
ATOM      1  N1   UDP     1      18.076  20.461  33.199    -0.40   -0.10   -0.211  2.311
ATOM      2  C2   UDP     1      18.358  21.720  32.747    -0.87   +0.28   +0.396  2.311
ATOM      3  N3   UDP     1      19.681  22.084  32.744    -0.50   -0.45   -0.440  2.311
ATOM      4  H3   UDP     1      19.900  23.036  32.419    +0.10   +0.73   +0.440  2.311
ATOM      5  C4   UDP     1      20.757  21.288  33.138    -0.77   +0.32   +0.396  2.311
ATOM      6  C5   UDP     1      20.397  19.982  33.593    -0.58   +0.00   +0.000  2.311
ATOM      7  C6   UDP     1      19.106  19.615  33.595    -0.51   +0.00   +0.000  2.311
ATOM      8  O2   UDP     1      17.472  22.491  32.375    -0.37   -0.26   -0.396  2.311
ATOM      9  O4   UDP     1      21.888  21.771  33.081    -0.27   -0.29   -0.396  2.311
ATOM     10  C1'  UDP     1      16.678  20.012  33.244    -0.68   +0.06   +0.324  2.311
ATOM     11  C2'  UDP     1      16.420  18.670  32.556    -0.65   -0.01   +0.113  2.311
ATOM     12  C3'  UDP     1      15.118  18.236  33.269    -0.69   -0.02   +0.113  2.311
ATOM     13  C4'  UDP     1      15.269  18.807  34.678    -0.55   +0.01   +0.113  2.311
ATOM     14  O4'  UDP     1      16.394  19.723  34.607    -0.07   -0.05   -0.227  2.311
ATOM     15  O2'  UDP     1      16.175  18.857  31.182    -0.21   +0.16   -0.537  2.311
ATOM     16  HO2'UDP     1      15.160  18.851  31.009    -0.25   -0.40   +0.424  2.311
ATOM     17  O3'  UDP     1      14.037  18.889  32.598    -0.19   +0.23   -0.537  2.311
ATOM     18  HO3'UDP     1      14.100  19.905  32.752    -0.41   -0.42   +0.424  2.311
ATOM     19  C5'  UDP     1      15.577  17.738  35.727    -0.35   +0.04   +0.113  2.311
ATOM     20  O5'  UDP     1      15.265  18.274  36.999    +0.05   -0.17   -0.368  2.311
ATOM     21  PA   UDP     1      15.981  18.217  38.403    -0.56   +0.43   +1.019  2.311
ATOM     22  O1A  UDP     1      17.432  18.480  38.185    -0.13   -0.08   -0.255  2.311
ATOM     23  O2A  UDP     1      15.236  19.101  39.354    -0.20   -0.11   -0.255  2.311
ATOM     24  O3A  UDP     1      15.744  16.656  38.636    +0.01   -0.22   -0.510  2.311
ATOM     25  PB   UDP     1      16.303  15.613  39.711    -0.67   +0.38   +1.019  2.311
ATOM     26  O1B  UDP     1      16.262  16.411  41.115    -0.60   -0.27   -0.255  2.311
ATOM     27  O2B  UDP     1      17.695  15.431  39.228    -0.12   -0.05   -0.255  2.311
ATOM     28  O3B  UDP     1      15.428  14.435  39.937    -0.08   -0.10   -0.255  2.311
TER
ENDMDL
MODEL       92
USER    Run = 92
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.359 A
USER
USER    Estimated Free Energy of Binding    =   -8.92 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +2.89e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.69 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -11.10 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.59 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
```

```
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.539656 19.734441 34.728197
USER    NEWDPF quat0-0.689836 -0.566725 0.450499 25.546722
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-130.87 -28.43 -171.32 27.28 8.87 -22.44 135.77
USER
USER                    Rank        x       y       z      vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.242  20.356  33.288   -0.37   -0.11  -0.211  2.359
ATOM      2  C2  UDP     1      18.519  21.569  32.723   -0.84   +0.27  +0.396  2.359
ATOM      3  N3  UDP     1      19.837  21.949  32.710   -0.51   -0.42  -0.440  2.359
ATOM      4  H3  UDP     1      20.052  22.868  32.300   +0.10   +0.55  +0.440  2.359
ATOM      5  C4  UDP     1      20.914  21.209  33.200   -0.76   +0.32  +0.396  2.359
ATOM      6  C5  UDP     1      20.559  19.948  33.772   -0.58   +0.00  +0.000  2.359
ATOM      7  C6  UDP     1      19.273  19.566  33.784   -0.50   +0.00  +0.000  2.359
ATOM      8  O2  UDP     1      17.631  22.290  32.261   -0.35   -0.24  -0.396  2.359
ATOM      9  O4  UDP     1      22.040  21.699  33.119   -0.26   -0.29  -0.396  2.359
ATOM     10  C1' UDP     1      16.848  19.895  33.349   -0.66   +0.07  +0.324  2.359
ATOM     11  C2' UDP     1      16.619  18.490  32.788   -0.58   +0.00  +0.113  2.359
ATOM     12  C3' UDP     1      15.308  18.109  33.514   -0.64   -0.01  +0.113  2.359
ATOM     13  C4' UDP     1      15.423  18.814  34.865   -0.57   +0.02  +0.113  2.359
ATOM     14  O4' UDP     1      16.540  19.734  34.728   -0.07   -0.07  -0.227  2.359
ATOM     15  O2' UDP     1      16.401  18.541  31.398   -0.22   +0.14  -0.537  2.359
ATOM     16  HO2'UDP     1      15.535  18.034  31.167   -0.34   -0.48  +0.424  2.359
ATOM     17  O3' UDP     1      14.233  18.680  32.763   -0.29   +0.18  -0.537  2.359
ATOM     18  HO3'UDP     1      14.190  19.693  32.939   -0.39   -0.32  +0.424  2.359
ATOM     19  C5' UDP     1      15.722  17.855  36.017   -0.34   +0.04  +0.113  2.359
ATOM     20  O5' UDP     1      15.522  18.557  37.230   -0.04   -0.17  -0.368  2.359
ATOM     21  PA  UDP     1      15.972  18.295  38.719   -0.53   +0.43  +1.019  2.359
ATOM     22  O1A UDP     1      17.449  18.480  38.787   -0.16   -0.07  -0.255  2.359
ATOM     23  O2A UDP     1      15.112  19.117  39.628   -0.25   -0.11  -0.255  2.359
ATOM     24  O3A UDP     1      15.622  16.738  38.716   +0.00   -0.22  -0.510  2.359
ATOM     25  PB  UDP     1      15.963  15.538  39.716   -0.67   +0.40  +1.019  2.359
ATOM     26  O1B UDP     1      15.535  16.087  41.174   -0.67   -0.21  -0.255  2.359
ATOM     27  O2B UDP     1      17.439  15.465  39.574   -0.14   -0.04  -0.255  2.359
ATOM     28  O3B UDP     1      15.130  14.324  39.526   -0.04   -0.11  -0.255  2.359
TER
ENDMDL
MODEL       80
USER    Run = 80
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.428 A
USER
USER    Estimated Free Energy of Binding    =   -8.73 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +4.00e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.68 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.91 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.77 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.264354 19.749050 34.748403
USER    NEWDPF quat0-0.636753 -0.548763 0.541668 23.855418
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-176.64 45.50 -32.26 16.31 -15.69 -5.13 142.41
USER
USER                    Rank        x       y       z      vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      17.903  20.465  33.279   -0.41   -0.10  -0.211  2.428
ATOM      2  C2  UDP     1      18.132  21.705  32.750   -0.88   +0.26  +0.396  2.428
ATOM      3  N3  UDP     1      19.439  22.119  32.710   -0.52   -0.45  -0.440  2.428
ATOM      4  H3  UDP     1      19.618  23.057  32.327   +0.10   +0.67  +0.440  2.428
ATOM      5  C4  UDP     1      20.550  21.389  33.139   -0.77   +0.34  +0.396  2.428
```

```
ATOM      6  C5  UDP     1      20.244  20.100  33.675    -0.60  +0.00  +0.000  2.428
ATOM      7  C6  UDP     1      18.969  19.685  33.713    -0.52  +0.00  +0.000  2.428
ATOM      8  O2  UDP     1      17.213  22.419  32.344    -0.37  -0.24  -0.396  2.428
ATOM      9  O4  UDP     1      21.660  21.911  33.040    -0.29  -0.30  -0.396  2.428
ATOM     10  C1' UDP     1      16.524  19.967  33.367    -0.67  +0.04  +0.324  2.428
ATOM     11  C2' UDP     1      16.312  18.577  32.762    -0.63  -0.01  +0.113  2.428
ATOM     12  C3' UDP     1      15.035  18.137  33.515    -0.69  -0.01  +0.113  2.428
ATOM     13  C4' UDP     1      15.176  18.796  34.886    -0.56  +0.02  +0.113  2.428
ATOM     14  O4' UDP     1      16.264  19.749  34.748    -0.07  -0.05  -0.227  2.428
ATOM     15  O2' UDP     1      16.047  18.672  31.383    -0.22  +0.20  -0.537  2.428
ATOM     16  HO2'UDP     1      15.803  17.742  31.014    -0.26  -0.50  +0.424  2.428
ATOM     17  O3' UDP     1      13.922  18.707  32.819    -0.29  +0.15  -0.537  2.428
ATOM     18  HO3'UDP     1      14.264  19.274  32.030    -0.21  -0.34  +0.424  2.428
ATOM     19  C5' UDP     1      15.535  17.804  35.993    -0.25  +0.04  +0.113  2.428
ATOM     20  O5' UDP     1      15.212  18.402  37.234    +0.01  -0.18  -0.368  2.428
ATOM     21  PA  UDP     1      15.866  18.342  38.668    -0.54  +0.44  +1.019  2.428
ATOM     22  O1A UDP     1      17.341  18.480  38.500    -0.14  -0.08  -0.255  2.428
ATOM     23  O2A UDP     1      15.159  19.318  39.556    -0.21  -0.10  -0.255  2.428
ATOM     24  O3A UDP     1      15.496  16.815  38.944    -0.03  -0.23  -0.510  2.428
ATOM     25  PB  UDP     1      16.112  15.696  39.906    -0.72  +0.42  +1.019  2.428
ATOM     26  O1B UDP     1      15.384  14.325  39.458    -0.03  -0.11  -0.255  2.428
ATOM     27  O2B UDP     1      15.627  16.164  41.229    -0.68  -0.23  -0.255  2.428
ATOM     28  O3B UDP     1      17.556  15.427  39.690    -0.13  -0.03  -0.255  2.428
TER
ENDMDL
MODEL       27
USER    Run = 27
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.268 A
USER
USER    Estimated Free Energy of Binding    =   -8.56 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +5.27e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.63 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.74 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.89 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.331560 19.472735 34.565318
USER    NEWDPF quat0-0.490819 -0.684766 0.538695 25.212334
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-131.49 50.61 -168.07 36.57 -13.24 1.80 131.03
USER
USER                    Rank        x       y       z       vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.039  20.309  33.246    -0.38  -0.10  -0.211  2.268
ATOM      2  C2  UDP     1      18.266  21.581  32.799    -0.85  +0.27  +0.396  2.268
ATOM      3  N3  UDP     1      19.561  22.029  32.866    -0.52  -0.46  -0.440  2.268
ATOM      4  H3  UDP     1      19.737  22.991  32.546    +0.05  +0.79  +0.440  2.268
ATOM      5  C4  UDP     1      20.662  21.305  33.326    -0.76  +0.35  +0.396  2.268
ATOM      6  C5  UDP     1      20.359  19.981  33.772    -0.58  +0.00  +0.000  2.268
ATOM      7  C6  UDP     1      19.097  19.533  33.705    -0.50  +0.00  +0.000  2.268
ATOM      8  O2  UDP     1      17.354  22.293  32.373    -0.36  -0.23  -0.396  2.268
ATOM      9  O4  UDP     1      21.761  21.858  33.327    -0.20  -0.36  -0.396  2.268
ATOM     10  C1' UDP     1      16.672  19.773  33.217    -0.67  +0.05  +0.324  2.268
ATOM     11  C2' UDP     1      16.538  18.413  32.527    -0.61  -0.01  +0.113  2.268
ATOM     12  C3' UDP     1      15.228  17.901  33.171    -0.64  -0.02  +0.113  2.268
ATOM     13  C4' UDP     1      15.264  18.487  34.582    -0.60  +0.02  +0.113  2.268
ATOM     14  O4' UDP     1      16.332  19.473  34.565    -0.06  -0.05  -0.227  2.268
ATOM     15  O2' UDP     1      16.359  18.577  31.140    -0.22  +0.17  -0.537  2.268
ATOM     16  HO2'UDP     1      15.535  18.041  30.834    -0.24  -0.56  +0.424  2.268
ATOM     17  O3' UDP     1      14.147  18.480  32.436    -0.31  +0.23  -0.537  2.268
```

```
ATOM     18  HO3'UDP     1      14.521  19.029  31.649    -0.25  -0.35  +0.424  2.268
ATOM     19  C5' UDP     1      15.580  17.445  35.655    -0.29  +0.04  +0.113  2.268
ATOM     20  O5' UDP     1      15.412  18.058  36.919    +0.06  -0.17  -0.368  2.268
ATOM     21  PA  UDP     1      16.233  18.008  38.265    -0.62  +0.41  +1.019  2.268
ATOM     22  O1A UDP     1      17.673  18.192  37.926    -0.15  -0.07  -0.255  2.268
ATOM     23  O2A UDP     1      15.608  18.955  39.240    -0.18  -0.11  -0.255  2.268
ATOM     24  O3A UDP     1      15.943  16.468  38.566    +0.00  -0.22  -0.510  2.268
ATOM     25  PB  UDP     1      16.424  15.469  39.718    -0.63  +0.36  +1.019  2.268
ATOM     26  O1B UDP     1      16.040  16.219  41.097    -0.67  -0.23  -0.255  2.268
ATOM     27  O2B UDP     1      17.891  15,464  39.492    -0.12  -0.02  -0.255  2.268
ATOM     28  O3B UDP     1      15.670  14.191  39.779    -0.05  -0.10  -0.255  2.268
TER
ENDMDL
MODEL       37
USER    Run = 37
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.337 A
USER
USER    Estimated Free Energy of Binding    =   -8.76 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +3.82e-07      [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.60 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.93 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.66 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.642481 19.664002 34.683293
USER    NEWDPF quat00.689785 0.638573 -0.341206 -21.274560
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-143.29 -16.74 -20.40 5.95 -28.82 6.66 151.74
USER
USER                    Rank        x       y       z       vdW    Elec     q     RMS
ATOM      1  N1  UDP     1      18.371  20.252  33.262    -0.36  -0.11  -0.211  2.337
ATOM      2  C2  UDP     1      18.727  21.475  32.765    -0.81  +0.28  +0.396  2.337
ATOM      3  N3  UDP     1      20.068  21.764  32.759    -0.54  -0.38  -0.440  2.337
ATOM      4  H3  UDP     1      20.343  22.689  32.400    +0.06  +0.49  +0.440  2.337
ATOM      5  C4  UDP     1      21.096  20.924  33.191    -0.74  +0.30  +0.396  2.337
ATOM      6  C5  UDP     1      20.659  19.659  33.692    -0.53  +0.00  +0.000  2.337
ATOM      7  C6  UDP     1      19.350  19.365  33.697    -0.48  +0.00  +0.000  2.337
ATOM      8  O2  UDP     1      17.888  22.281  32.358    -0.33  -0.26  -0.396  2.337
ATOM      9  O4  UDP     1      22.252  21.340  33.125    -0.24  -0.30  -0.396  2.337
ATOM     10  C1' UDP     1      16.950  19.885  33.312    -0.66  +0.08  +0.324  2.337
ATOM     11  C2' UDP     1      16.620  18.534  32.673    -0.60  +0.00  +0.113  2.337
ATOM     12  C3' UDP     1      15.292  18.202  33.391    -0.66  -0.01  +0.113  2.337
ATOM     13  C4' UDP     1      15.466  18.816  34.779    -0.57  +0.02  +0.113  2.337
ATOM     14  O4' UDP     1      16.642  19.664  34.683    -0.06  -0.07  -0.227  2.337
ATOM     15  O2' UDP     1      16.394  18.683  31.291    -0.22  +0.13  -0.537  2.337
ATOM     16  HO2'UDP     1      15.610  18.081  31.004    -0.31  -0.47  +0.424  2.337
ATOM     17  O3' UDP     1      14.253  18.888  32.688    -0.24  +0.22  -0.537  2.337
ATOM     18  HO3'UDP     1      14.399  19.905  32.765    -0.37  -0.36  +0.424  2.337
ATOM     19  C5' UDP     1      15.707  17.771  35.870    -0.36  +0.04  +0.113  2.337
ATOM     20  O5' UDP     1      15.214  18.294  37.088    +0.06  -0.17  -0.368  2.337
ATOM     21  PA  UDP     1      15.799  18.368  38.552    -0.54  +0.44  +1.019  2.337
ATOM     22  O1A UDP     1      17.282  18.480  38.442    -0.13  -0.08  -0.255  2.337
ATOM     23  O2A UDP     1      15.062  19.430  39.306    -0.22  -0.10  -0.255  2.337
ATOM     24  O3A UDP     1      15.399  16.877  38.955    +0.00  -0.23  -0.510  2.337
ATOM     25  PB  UDP     1      16.080  15.778  39.895    -0.73  +0.43  +1.019  2.337
ATOM     26  O1B UDP     1      15.467  14.371  39.390    -0.02  -0.11  -0.255  2.337
ATOM     27  O2B UDP     1      15.536  16.165  41.221    -0.68  -0.23  -0.255  2.337
ATOM     28  O3B UDP     1      17.545  15.626  39.701    -0.18  -0.03  -0.255  2.337
TER
```

```
ENDMDL
MODEL       83
USER    Run = 83
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.261 A
USER
USER    Estimated Free Energy of Binding    =   -8.49 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +5.99e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.46 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.67 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.79 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.357985 19.606004 34.816153
USER    NEWDPF quat0-0.457891 -0.473843 0.752202 19.873212
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-102.27 -10.98 18.83 69.93 -8.93 -8.56 143.76
USER
USER                    Rank         x       y       z       vdW    Elec       q     RMS
ATOM      1  N1  UDP     1      17.847  20.520  33.298    -0.42   -0.10  -0.211   2.261
ATOM      2  C2  UDP     1      17.991  21.811  32.873    -0.89   +0.27  +0.396   2.261
ATOM      3  N3  UDP     1      19.276  22.280  32.771    -0.52   -0.49  -0.440   2.261
ATOM      4  H3  UDP     1      19.392  23.256  32.466    +0.09   +0.81  +0.440   2.261
ATOM      5  C4  UDP     1      20.441  21.560  33.040    -0.78   +0.35  +0.396   2.261
ATOM      6  C5  UDP     1      20.223  20.216  33.473    -0.61   +0.00  +0.000   2.261
ATOM      7  C6  UDP     1      18.970  19.747  33.571    -0.52   +0.00  +0.000   2.261
ATOM      8  O2  UDP     1      17.018  22.522  32.609    -0.35   -0.26  -0.396   2.261
ATOM      9  O4  UDP     1      21.522  22.133  32.905    -0.18   -0.29  -0.396   2.261
ATOM     10  C1' UDP     1      16.497  19.961  33.445    -0.66   +0.04  +0.324   2.261
ATOM     11  C2' UDP     1      16.282  18.624  32.730    -0.64   -0.01  +0.113   2.261
ATOM     12  C3' UDP     1      15.086  18.065  33.535    -0.68   -0.01  +0.113   2.261
ATOM     13  C4' UDP     1      15.316  18.601  34.948    -0.57   +0.02  +0.113   2.261
ATOM     14  O4' UDP     1      16.358  19.606  34.816    -0.06   -0.06  -0.227   2.261
ATOM     15  O2' UDP     1      15.903  18.835  31.391    -0.19   +0.21  -0.537   2.261
ATOM     16  HO2'UDP     1      14.882  18.739  31.303    -0.21   -0.42  +0.424   2.261
ATOM     17  O3' UDP     1      13.902  18.651  32.985    -0.32   +0.11  -0.537   2.261
ATOM     18  HO3'UDP     1      13.966  19.677  33.045    -0.44   -0.31  +0.424   2.261
ATOM     19  C5' UDP     1      15.797  17.527  35.924    -0.30   +0.04  +0.113   2.261
ATOM     20  O5' UDP     1      15.528  17.981  37.236    +0.01   -0.17  -0.368   2.261
ATOM     21  PA  UDP     1      16.241  17.761  38.626    -0.67   +0.41  +1.019   2.261
ATOM     22  O1A UDP     1      17.687  18.081  38.451    -0.20   -0.05  -0.255   2.261
ATOM     23  O2A UDP     1      15.474  18.500  39.678    -0.24   -0.12  -0.255   2.261
ATOM     24  O3A UDP     1      16.039  16.179  38.656    -0.01   -0.22  -0.510   2.261
ATOM     25  PB  UDP     1      15.854  15.121  39.841    -0.63   +0.38  +1.019   2.261
ATOM     26  O1B UDP     1      17.108  14.114  39.690    +0.11   -0.05  -0.255   2.261
ATOM     27  O2B UDP     1      14.581  14.471  39.442    -0.01   -0.09  -0.255   2.261
ATOM     28  O3B UDP     1      16.010  15.692  41.204    -0.60   -0.19  -0.255   2.261
TER
ENDMDL
MODEL       65
USER    Run = 65
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.304 A
USER
USER    Estimated Free Energy of Binding    =   -8.71 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +4.12e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.45 kcal/mol  [=(1)+(2)]
```

```
USER
USER    (1) Final Intermolecular Energy     =  -10.89 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.56 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.670987 19.529452 34.985959
USER    NEWDPF quat0-0.609578 -0.251836 0.751660 12.309821
USER    NEWDPF ndihe7
USER    NEWDPF dihe0174.86 35.30 170.27 1.85 94.80 -103.65 115.10
USER
USER                    Rank       x       y       z      vdW     Elec       q     RMS
ATOM      1  N1  UDP     1      18.083  20.325  33.334   -0.38   -0.10   -0.211  2.304
ATOM      2  C2  UDP     1      18.319  21.606  32.917   -0.85   +0.28   +0.396  2.304
ATOM      3  N3  UDP     1      19.629  21.940  32.687   -0.53   -0.41   -0.440  2.304
ATOM      4  H3  UDP     1      19.816  22.907  32.388   +0.07   +0.65   +0.440  2.304
ATOM      5  C4  UDP     1      20.733  21.096  32.819   -0.75   +0.27   +0.396  2.304
ATOM      6  C5  UDP     1      20.419  19.770  33.251   -0.56   +0.00   +0.000  2.304
ATOM      7  C6  UDP     1      19.140  19.432  33.474   -0.48   +0.00   +0.000  2.304
ATOM      8  O2  UDP     1      17.406  22.420  32.770   -0.33   -0.29   -0.396  2.304
ATOM      9  O4  UDP     1      21.849  21.556  32.580   -0.14   -0.18   -0.396  2.304
ATOM     10  C1' UDP     1      16.704  19.905  33.614   -0.64   +0.07   +0.324  2.304
ATOM     11  C2' UDP     1      16.275  18.619  32.904   -0.62   +0.00   +0.113  2.304
ATOM     12  C3' UDP     1      15.116  18.166  33.822   -0.65   +0.00   +0.113  2.304
ATOM     13  C4' UDP     1      15.548  18.635  35.210   -0.55   +0.03   +0.113  2.304
ATOM     14  O4' UDP     1      16.671  19.529  34.986   -0.05   -0.08   -0.227  2.304
ATOM     15  O2' UDP     1      15.784  18.905  31.616   -0.27   +0.21   -0.537  2.304
ATOM     16  HO2'UDP     1      15.535  18.027  31.140   -0.35   -0.48   +0.424  2.304
ATOM     17  O3' UDP     1      13.951  18.887  33.410   -0.22   +0.09   -0.537  2.304
ATOM     18  HO3'UDP     1      14.224  19.643  32.767   -0.35   -0.32   +0.424  2.304
ATOM     19  C5' UDP     1      16.010  17.490  36.112   -0.40   +0.04   +0.113  2.304
ATOM     20  O5' UDP     1      16.561  18.057  37.285   -0.03   -0.15   -0.368  2.304
ATOM     21  PA  UDP     1      16.153  18.005  38.808   -0.70   +0.42   +1.019  2.304
ATOM     22  O1A UDP     1      17.382  18.249  39.616   -0.14   -0.06   -0.255  2.304
ATOM     23  O2A UDP     1      14.977  18.907  39.017   -0.21   -0.12   -0.255  2.304
ATOM     24  O3A UDP     1      15.798  16.450  38.822   -0.02   -0.22   -0.510  2.304
ATOM     25  PB  UDP     1      16.010  15.288  39.900   -0.66   +0.39   +1.019  2.304
ATOM     26  O1B UDP     1      15.889  16.031  41.330   -0.67   -0.25   -0.255  2.304
ATOM     27  O2B UDP     1      17.410  14.888  39.610   +0.00   -0.04   -0.255  2.304
ATOM     28  O3B UDP     1      14.929  14.270  39.927   -0.06   -0.10   -0.255  2.304
TER
ENDMDL
MODEL       14
USER    Run = 14
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.451 A
USER
USER    Estimated Free Energy of Binding    =   -8.42 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +6.69e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.42 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.60 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.82 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran017.100220 19.724175 34.926891
USER    NEWDPF quat00.896782 0.345563 -0.276348 -20.343759
USER    NEWDPF ndihe7
```

```
USER    NEWDPF dihe0179.92 79.45 -26.55 -16.81 -42.81 3.24 -180.00
USER
USER                    Rank      x       y       z      vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.694  20.131  33.299   -0.34  -0.11  -0.211  2.451
ATOM      2  C2  UDP     1      19.052  21.300  32.688   -0.77  +0.27  +0.396  2.451
ATOM      3  N3  UDP     1      20.396  21.516  32.524   -0.51  -0.30  -0.440  2.451
ATOM      4  H3  UDP     1      20.674  22.402  32.079   +0.08  +0.21  +0.440  2.451
ATOM      5  C4  UDP     1      21.424  20.651  32.904   -0.72  +0.26  +0.396  2.451
ATOM      6  C5  UDP     1      20.984  19.444  33.531   -0.51  +0.00  +0.000  2.451
ATOM      7  C6  UDP     1      19.671  19.222  33.690   -0.47  +0.00  +0.000  2.451
ATOM      8  O2  UDP     1      18.212  22.123  32.316   -0.30  -0.27  -0.396  2.451
ATOM      9  O4  UDP     1      22.585  21.000  32.692   -0.24  -0.25  -0.396  2.451
ATOM     10  C1' UDP     1      17.271  19.844  33.519   -0.61  +0.10  +0.324  2.451
ATOM     11  C2' UDP     1      16.813  18.475  33.009   -0.53  +0.01  +0.113  2.451
ATOM     12  C3' UDP     1      15.554  18.259  33.881   -0.59  +0.00  +0.113  2.451
ATOM     13  C4' UDP     1      15.903  18.947  35.200   -0.55  +0.03  +0.113  2.451
ATOM     14  O4' UDP     1      17.100  19.724  34.927   -0.05  -0.10  -0.227  2.451
ATOM     15  O2' UDP     1      16.449  18.550  31.651   -0.21  +0.11  -0.537  2.451
ATOM     16 HO2'UDP     1      16.098  17.634  31.338   -0.22  -0.34  +0.424  2.451
ATOM     17  O3' UDP     1      14.479  18.955  33.244   -0.22  +0.14  -0.537  2.451
ATOM     18 HO3'UDP     1      14.616  18.939  32.223   -0.09  -0.24  +0.424  2.451
ATOM     19  C5' UDP     1      16.209  17.961  36.327   -0.46  +0.04  +0.113  2.451
ATOM     20  O5' UDP     1      15.331  18.241  37.401   +0.04  -0.17  -0.368  2.451
ATOM     21  PA  UDP     1      15.526  18.335  38.963   -0.69  +0.46  +1.019  2.451
ATOM     22  O1A UDP     1      16.986  18.480  39.231   -0.17  -0.09  -0.255  2.451
ATOM     23  O2A UDP     1      14.600  19.383  39.497   -0.29  -0.11  -0.255  2.451
ATOM     24  O3A UDP     1      15.068  16.838  39.267   -0.05  -0.23  -0.510  2.451
ATOM     25  PB  UDP     1      15.770  15.608  40.009   -0.72  +0.42  +1.019  2.451
ATOM     26  O1B UDP     1      14.899  14.318  39.578   -0.04  -0.10  -0.255  2.451
ATOM     27  O2B UDP     1      15.542  15.969  41.431   -0.71  -0.24  -0.255  2.451
ATOM     28  O3B UDP     1      17.140  15.298  39.525   -0.10  -0.06  -0.255  2.451
TER
ENDMDL
MODEL       99
USER    Run = 99
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.336 A
USER
USER    Estimated Free Energy of Binding    =   -8.47 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +6.23e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.36 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.65 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.71 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.837146 19.319611 35.006964
USER    NEWDPF quat0-0.287528 -0.036292 0.957084 6.817381
USER    NEWDPF ndihe7
USER    NEWDPF dihe0179.27 74.01 -73.43 -63.66 -99.15 70.88 172.83
USER
USER                    Rank      x       y       z      vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.200  20.203  33.359   -0.36  -0.10  -0.211  2.336
ATOM      2  C2  UDP     1      18.479  21.505  33.049   -0.82  +0.29  +0.396  2.336
ATOM      3  N3  UDP     1      19.791  21.800  32.777   -0.55  -0.39  -0.440  2.336
ATOM      4  H3  UDP     1      20.011  22.781  32.558   +0.03  +0.65  +0.440  2.336
ATOM      5  C4  UDP     1      20.855  20.897  32.768   -0.73  +0.25  +0.396  2.336
ATOM      6  C5  UDP     1      20.497  19.552  33.093   -0.53  +0.00  +0.000  2.336
ATOM      7  C6  UDP     1      19.216  19.253  33.355   -0.47  +0.00  +0.000  2.336
ATOM      8  O2  UDP     1      17.602  22.371  33.029   -0.28  -0.32  -0.396  2.336
ATOM      9  O4  UDP     1      21.979  21.327  32.510   -0.20  -0.19  -0.396  2.336
```

```
ATOM     10  C1' UDP     1      16.818  19.822  33.676    -0.62  +0.08  +0.324  2.336
ATOM     11  C2' UDP     1      16.288  18.630  32.876    -0.62  +0.00  +0.113  2.336
ATOM     12  C3' UDP     1      15.157  18.145  33.812    -0.65  +0.00  +0.113  2.336
ATOM     13  C4' UDP     1      15.683  18.461  35.211    -0.54  +0.03  +0.113  2.336
ATOM     14  O4' UDP     1      16.837  19.320  35.007    -0.03  -0.08  -0.227  2.336
ATOM     15  O2' UDP     1      15.746  19.059  31.649    -0.28  +0.19  -0.537  2.336
ATOM     16  HO2'UDP     1      15.361  18.251  31.141    -0.25  -0.48  +0.424  2.336
ATOM     17  O3' UDP     1      14.010  18.954  33.535    -0.18  +0.08  -0.537  2.336
ATOM     18  HO3'UDP     1      14.056  19.295  32.564    -0.26  -0.27  +0.424  2.336
ATOM     19  C5' UDP     1      16.133  17.215  35.975    -0.37  +0.04  +0.113  2.336
ATOM     20  O5' UDP     1      15.535  17.253  37.257    +0.26  -0.17  -0.368  2.336
ATOM     21  PA  UDP     1      15.745  18.170  38.524    -0.58  +0.44  +1.019  2.336
ATOM     22  O1A UDP     1      17.206  18.434  38.656    -0.14  -0.08  -0.255  2.336
ATOM     23  O2A UDP     1      14.819  19.342  38.422    +0.01  -0.12  -0.255  2.336
ATOM     24  O3A UDP     1      15.296  17.070  39.589    -0.16  -0.24  -0.510  2.336
ATOM     25  PB  UDP     1      16.020  15.783  40.203    -0.79  +0.47  +1.019  2.336
ATOM     26  O1B UDP     1      15.432  15.660  41.703    -0.68  -0.24  -0.255  2.336
ATOM     27  O2B UDP     1      17.435  16.232  40.207    -0.48  -0.07  -0.255  2.336
ATOM     28  O3B UDP     1      15.642  14.500  39.559    -0.04  -0.10  -0.255  2.336
TER
ENDMDL
MODEL       89
USER    Run = 89
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.343 A
USER
USER    Estimated Free Energy of Binding    =   -8.33 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +7.88e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.35 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.51 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.85 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran017.054940 19.477433 34.899250
USER    NEWDPF quat00.673805 0.287903 -0.680513 -10.385254
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-157.20 94.24 8.30 -47.60 -85.48 50.85 179.66
USER
USER                    Rank         x       y       z       vdW    Elec       q     RMS
ATOM      1  N1  UDP     1      18.496  20.235  33.255    -0.35  -0.11  -0.211  2.343
ATOM      2  C2  UDP     1      18.781  21.510  32.850    -0.81  +0.29  +0.396  2.343
ATOM      3  N3  UDP     1      20.102  21.797  32.623    -0.54  -0.36  -0.440  2.343
ATOM      4  H3  UDP     1      20.326  22.759  32.333    +0.07  +0.48  +0.440  2.343
ATOM      5  C4  UDP     1      21.173  20.910  32.747    -0.74  +0.25  +0.396  2.343
ATOM      6  C5  UDP     1      20.809  19.593  33.165    -0.54  +0.00  +0.000  2.343
ATOM      7  C6  UDP     1      19.518  19.301  33.385    -0.48  +0.00  +0.000  2.343
ATOM      8  O2  UDP     1      17.899  22.360  32.711    -0.29  -0.31  -0.396  2.343
ATOM      9  O4  UDP     1      22.306  21.330  32.511    -0.20  -0.19  -0.396  2.343
ATOM     10  C1' UDP     1      17.102  19.865  33.531    -0.63  +0.09  +0.324  2.343
ATOM     11  C2' UDP     1      16.625  18.603  32.809    -0.59  +0.00  +0.113  2.343
ATOM     12  C3' UDP     1      15.449  18.185  33.722    -0.61  +0.00  +0.113  2.343
ATOM     13  C4' UDP     1      15.898  18.624  35.115    -0.53  +0.03  +0.113  2.343
ATOM     14  O4' UDP     1      17.055  19.477  34.899    -0.04  -0.09  -0.227  2.343
ATOM     15  O2' UDP     1      16.145  18.920  31.523    -0.25  +0.14  -0.537  2.343
ATOM     16  HO2'UDP     1      15.461  18.210  31.227    -0.28  -0.43  +0.424  2.343
ATOM     17  O3' UDP     1      14.312  18.954  33.318    -0.21  +0.13  -0.537  2.343
ATOM     18  HO3'UDP     1      14.225  18.926  32.293    -0.16  -0.24  +0.424  2.343
ATOM     19  C5' UDP     1      16.317  17.454  36.005    -0.40  +0.04  +0.113  2.343
ATOM     20  O5' UDP     1      15.535  17.503  37.184    +0.15  -0.17  -0.368  2.343
ATOM     21  PA  UDP     1      15.723  18.213  38.580    -0.59  +0.44  +1.019  2.343
```

```
ATOM     22  O1A UDP     1      17.185  18.409  38.796    -0.16  -0.08  -0.255  2.343
ATOM     23  O2A UDP     1      14.832  19.415  38.627    -0.06  -0.11  -0.255  2.343
ATOM     24  O3A UDP     1      15.209  16.980  39.452    -0.12  -0.23  -0.510  2.343
ATOM     25  PB  UDP     1      15.954  15.754  40.159    -0.78  +0.45  +1.019  2.343
ATOM     26  O1B UDP     1      15.139  14.446  39.676    -0.06  -0.10  -0.255  2.343
ATOM     27  O2B UDP     1      15.699  16.058  41.590    -0.72  -0.29  -0.255  2.343
ATOM     28  O3B UDP     1      17.339  15.516  39.679    -0.16  -0.05  -0.255  2.343
TER
ENDMDL
MODEL       75
USER    Run = 75
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.190 A
USER
USER    Estimated Free Energy of Binding    =   -8.35 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +7.52e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.34 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.53 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.81 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.649808 19.351573 34.884284
USER    NEWDPF quat00.238273 0.242155 -0.940525 -7.710898
USER    NEWDPF ndihe7
USER    NEWDPF dihe0162.51 45.31 -179.82 136.56 -34.17 0.93 124.87
USER
USER                    Rank        x       y       z       vdW    Elec       q     RMS
ATOM      1  N1  UDP     1      18.047  20.259  33.278    -0.38  -0.10  -0.211  2.190
ATOM      2  C2  UDP     1      18.316  21.566  32.981    -0.84  +0.28  +0.396  2.190
ATOM      3  N3  UDP     1      19.631  21.879  32.746    -0.54  -0.40  -0.440  2.190
ATOM      4  H3  UDP     1      19.844  22.864  32.537    +0.04  +0.71  +0.440  2.190
ATOM      5  C4  UDP     1      20.707  20.990  32.764    -0.74  +0.26  +0.396  2.190
ATOM      6  C5  UDP     1      20.358  19.639  33.074    -0.54  +0.00  +0.000  2.190
ATOM      7  C6  UDP     1      19.074  19.323  33.299    -0.48  +0.00  +0.000  2.190
ATOM      8  O2  UDP     1      17.429  22.420  32.939    -0.30  -0.31  -0.396  2.190
ATOM      9  O4  UDP     1      21.832  21.436  32.538    -0.16  -0.18  -0.396  2.190
ATOM     10  C1' UDP     1      16.661  19.859  33.555    -0.64  +0.06  +0.324  2.190
ATOM     11  C2' UDP     1      16.169  18.663  32.736    -0.65  -0.01  +0.113  2.190
ATOM     12  C3' UDP     1      15.019  18.160  33.638    -0.68  -0.01  +0.113  2.190
ATOM     13  C4' UDP     1      15.502  18.477  35.053    -0.56  +0.03  +0.113  2.190
ATOM     14  O4' UDP     1      16.650  19.352  34.884    -0.04  -0.07  -0.227  2.190
ATOM     15  O2' UDP     1      15.656  19.090  31.496    -0.23  +0.22  -0.537  2.190
ATOM     16  HO2'UDP     1      15.558  18.281  30.868    -0.28  -0.45  +0.424  2.190
ATOM     17  O3' UDP     1      13.870  18.955  33.333    -0.22  +0.10  -0.537  2.190
ATOM     18  HO3'UDP     1      14.118  19.662  32.626    -0.35  -0.35  +0.424  2.190
ATOM     19  C5' UDP     1      15.946  17.234  35.825    -0.35  +0.04  +0.113  2.190
ATOM     20  O5' UDP     1      16.337  17.645  37.122    +0.01  -0.15  -0.368  2.190
ATOM     21  PA  UDP     1      17.525  17.236  38.076    -0.63  +0.28  +1.019  2.190
ATOM     22  O1A UDP     1      18.643  16.742  37.223    +0.08  -0.09  -0.255  2.190
ATOM     23  O2A UDP     1      17.796  18.371  39.013    -0.21  -0.03  -0.255  2.190
ATOM     24  O3A UDP     1      16.769  16.000  38.744    -0.03  -0.18  -0.510  2.190
ATOM     25  PB  UDP     1      15.718  15.879  39.943    -0.73  +0.44  +1.019  2.190
ATOM     26  O1B UDP     1      14.699  17.113  39.721    -0.15  -0.12  -0.255  2.190
ATOM     27  O2B UDP     1      16.601  16.105  41.115    -0.56  -0.24  -0.255  2.190
ATOM     28  O3B UDP     1      14.849  14.676  39.880    +0.00  -0.08  -0.255  2.190
TER
ENDMDL
MODEL       34
USER    Run = 34
USER    Cluster Rank = 1
```

```
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.097 A
USER
USER    Estimated Free Energy of Binding    =   -8.20 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +9.82e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.33 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.38 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.96 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.582017 19.303584 34.740441
USER    NEWDPF quat0-0.262934 -0.600146 0.755440 8.281891
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-95.21 12.27 76.12 136.23 -39.68 40.94 148.63
USER
USER                    Rank         x       y       z       vdW    Elec       q     RMS
ATOM      1  N1  UDP     1      18.079  20.184  33.211    -0.37  -0.10  -0.211  2.097
ATOM      2  C2  UDP     1      18.387  21.485  32.927    -0.83  +0.27  +0.396  2.097
ATOM      3  N3  UDP     1      19.717  21.776  32.764    -0.54  -0.39  -0.440  2.097
ATOM      4  H3  UDP     1      19.958  22.757  32.565    +0.03  +0.64  +0.440  2.097
ATOM      5  C4  UDP     1      20.776  20.870  32.842    -0.73  +0.26  +0.396  2.097
ATOM      6  C5  UDP     1      20.388  19.526  33.135    -0.53  +0.00  +0.000  2.097
ATOM      7  C6  UDP     1      19.089  19.231  33.290    -0.47  +0.00  +0.000  2.097
ATOM      8  O2  UDP     1      17.517  22.354  32.836    -0.31  -0.30  -0.396  2.097
ATOM      9  O4  UDP     1      21.919  21.296  32.678    -0.22  -0.22  -0.396  2.097
ATOM     10  C1' UDP     1      16.674  19.807  33.413    -0.65  +0.06  +0.324  2.097
ATOM     11  C2' UDP     1      16.208  18.618  32.570    -0.66  -0.01  +0.113  2.097
ATOM     12  C3' UDP     1      15.002  18.136  33.409    -0.70  -0.01  +0.113  2.097
ATOM     13  C4' UDP     1      15.412  18.448  34.848    -0.57  +0.02  +0.113  2.097
ATOM     14  O4' UDP     1      16.582  19.304  34.740    -0.04  -0.07  -0.227  2.097
ATOM     15  O2' UDP     1      15.770  19.049  31.304    -0.17  +0.21  -0.537  2.097
ATOM     16  HO2'UDP     1      14.756  19.225  31.332    -0.30  -0.36  +0.424  2.097
ATOM     17  O3' UDP     1      13.885  18.949  33.040    -0.27  +0.14  -0.537  2.097
ATOM     18  HO3'UDP     1      14.208  19.905  32.835    -0.40  -0.39  +0.424  2.097
ATOM     19  C5' UDP     1      15.793  17.201  35.645    -0.31  +0.04  +0.113  2.097
ATOM     20  O5' UDP     1      15.583  17.480  37.016    +0.14  -0.17  -0.368  2.097
ATOM     21  PA  UDP     1      16.541  17.904  38.195    -0.62  +0.39  +1.019  2.097
ATOM     22  O1A UDP     1      17.777  18.479  37.591    -0.14  -0.08  -0.255  2.097
ATOM     23  O2A UDP     1      15.767  18.746  39.161    -0.16  -0.11  -0.255  2.097
ATOM     24  O3A UDP     1      16.829  16.419  38.703    -0.05  -0.18  -0.510  2.097
ATOM     25  PB  UDP     1      16.037  15.420  39.668    -0.65  +0.40  +1.019  2.097
ATOM     26  O1B UDP     1      16.000  16.175  41.096    -0.67  -0.23  -0.255  2.097
ATOM     27  O2B UDP     1      16.961  14.258  39.690    +0.04  -0.05  -0.255  2.097
ATOM     28  O3B UDP     1      14.606  15.233  39.320    +0.09  -0.09  -0.255  2.097
TER
ENDMDL
MODEL       20
USER    Run = 20
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.190 A
USER
USER    Estimated Free Energy of Binding    =   -8.37 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +7.36e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.31 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.55 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.77 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
```

```
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.600663 19.139251 34.607528
USER    NEWDPF quat0-0.372510 0.542970 -0.752609 -7.650237
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-104.31 14.83 -107.06 15.47 -94.66 40.90 152.31
USER
USER                    Rank      x       y       z      vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.075  20.143  33.132   -0.37  -0.09  -0.211  2.190
ATOM      2  C2  UDP     1      18.384  21.463  32.956   -0.82  +0.27  +0.396  2.190
ATOM      3  N3  UDP     1      19.713  21.760  32.794   -0.54  -0.39  -0.440  2.190
ATOM      4  H3  UDP     1      19.956  22.754  32.677   +0.03  +0.69  +0.440  2.190
ATOM      5  C4  UDP     1      20.768  20.846  32.773   -0.73  +0.25  +0.396  2.190
ATOM      6  C5  UDP     1      20.377  19.484  32.955   -0.52  +0.00  +0.000  2.190
ATOM      7  C6  UDP     1      19.079  19.182  33.109   -0.47  +0.00  +0.000  2.190
ATOM      8  O2  UDP     1      17.518  22.340  32.958   -0.30  -0.31  -0.396  2.190
ATOM      9  O4  UDP     1      21.910  21.280  32.624   -0.22  -0.21  -0.396  2.190
ATOM     10  C1' UDP     1      16.671  19.756  33.327   -0.65  +0.05  +0.324  2.190
ATOM     11  C2' UDP     1      16.183  18.646  32.394   -0.68  -0.02  +0.113  2.190
ATOM     12  C3' UDP     1      14.989  18.099  33.210   -0.70  -0.02  +0.113  2.190
ATOM     13  C4' UDP     1      15.428  18.283  34.662   -0.57  +0.02  +0.113  2.190
ATOM     14  O4' UDP     1      16.601  19.139  34.608   -0.02  -0.06  -0.227  2.190
ATOM     15  O2' UDP     1      15.724  19.189  31.178   -0.10  +0.21  -0.537  2.190
ATOM     16  HO2'UDP     1      14.695  19.223  31.183   -0.35  -0.39  +0.424  2.190
ATOM     17  O3' UDP     1      13.870  18.945  32.934   -0.23  +0.16  -0.537  2.190
ATOM     18  HO3'UDP     1      14.199  19.907  32.765   -0.40  -0.40  +0.424  2.190
ATOM     19  C5' UDP     1      15.816  16.969  35.341   -0.37  +0.04  +0.113  2.190
ATOM     20  O5' UDP     1      15.552  17.100  36.725   +0.25  -0.17  -0.368  2.190
ATOM     21  PA  UDP     1      16.459  17.421  37.975   -0.55  +0.40  +1.019  2.190
ATOM     22  O1A UDP     1      17.794  16.803  37.739   -0.04  -0.08  -0.255  2.190
ATOM     23  O2A UDP     1      16.397  18.893  38.244   +0.11  -0.11  -0.255  2.190
ATOM     24  O3A UDP     1      15.626  16.531  39.004   -0.05  -0.22  -0.510  2.190
ATOM     25  PB  UDP     1      15.999  15.820  40.387   -0.80  +0.51  +1.019  2.190
ATOM     26  O1B UDP     1      15.099  16.580  41.493   -0.45  -0.30  -0.255  2.190
ATOM     27  O2B UDP     1      17.434  16.180  40.511   -0.51  -0.09  -0.255  2.190
ATOM     28  O3B UDP     1      15.571  14.401  40.484   -0.15  -0.10  -0.255  2.190
TER
ENDMDL
MODEL       7
USER    Run = 7
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.106 A
USER
USER    Estimated Free Energy of Binding    =   -8.01 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.34e-06     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.14 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.19 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.95 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.771562 19.240141 34.663676
USER    NEWDPF quat0-0.276654 -0.688269 0.670632 9.784323
USER    NEWDPF ndihe7
USER    NEWDPF dihe0179.04 77.47 173.47 135.89 -39.09 46.20 144.65
USER
USER                    Rank      x       y       z      vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.311  20.117  33.175   -0.35  -0.10  -0.211  2.106
```

```
ATOM      2  C2  UDP     1      18.620  21.418  32.890    -0.81  +0.28  +0.396  2.106
ATOM      3  N3  UDP     1      19.953  21.715  32.766    -0.54  -0.38  -0.440  2.106
ATOM      4  H3  UDP     1      20.195  22.696  32.567    +0.03  +0.60  +0.440  2.106
ATOM      5  C4  UDP     1      21.014  20.815  32.885    -0.73  +0.26  +0.396  2.106
ATOM      6  C5  UDP     1      20.624  19.471  33.175    -0.52  +0.00  +0.000  2.106
ATOM      7  C6  UDP     1      19.323  19.171  33.293    -0.46  +0.00  +0.000  2.106
ATOM      8  O2  UDP     1      17.749  22.281  32.765    -0.31  -0.30  -0.396  2.106
ATOM      9  O4  UDP     1      22.159  21.247  32.752    -0.23  -0.23  -0.396  2.106
ATOM     10  C1' UDP     1      16.902  19.734  33.336    -0.64  +0.07  +0.324  2.106
ATOM     11  C2' UDP     1      16.469  18.535  32.489    -0.64  -0.01  +0.113  2.106
ATOM     12  C3' UDP     1      15.240  18.053  33.293    -0.66  -0.02  +0.113  2.106
ATOM     13  C4' UDP     1      15.604  18.379  34.741    -0.55  +0.02  +0.113  2.106
ATOM     14  O4' UDP     1      16.772  19.240  34.664    -0.02  -0.07  -0.227  2.106
ATOM     15  O2' UDP     1      16.069  18.955  31.205    -0.23  +0.16  -0.537  2.106
ATOM     16  HO2'UDP     1      15.750  18.141  30.661    -0.30  -0.45  +0.424  2.106
ATOM     17  O3' UDP     1      14.130  18.857  32.883    -0.26  +0.18  -0.537  2.106
ATOM     18  HO3'UDP     1      14.258  19.144  31.902    -0.23  -0.34  +0.424  2.106
ATOM     19  C5' UDP     1      15.967  17.140  35.560    -0.37  +0.04  +0.113  2.106
ATOM     20  O5' UDP     1      15.800  17.459  36.928    +0.08  -0.16  -0.368  2.106
ATOM     21  PA  UDP     1      16.783  17.981  38.046    -0.62  +0.37  +1.019  2.106
ATOM     22  O1A UDP     1      17.949  18.615  37.366    -0.12  -0.09  -0.255  2.106
ATOM     23  O2A UDP     1      16.001  18.802  39.024    -0.10  -0.11  -0.255  2.106
ATOM     24  O3A UDP     1      17.191  16.535  38.582    -0.07  -0.15  -0.510  2.106
ATOM     25  PB  UDP     1      16.517  15.522  39.619    -0.63  +0.35  +1.019  2.106
ATOM     26  O1B UDP     1      14.927  15.708  39.398    +0.03  -0.09  -0.255  2.106
ATOM     27  O2B UDP     1      16.960  16.105  40.911    -0.49  -0.21  -0.255  2.106
ATOM     28  O3B UDP     1      16.759  14.087  39.322    +0.01  -0.09  -0.255  2.106
TER
ENDMDL
MODEL       59
USER    Run = 59
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure      = 2.112 A
USER
USER    Estimated Free Energy of Binding    =   -8.37 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +7.26e-07      [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.13 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.55 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.58 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.789117 19.079734 34.943430
USER    NEWDPF quat00.532175 0.338229 0.776138 5.198164
USER    NEWDPF ndihe7
USER    NEWDPF dihe0163.86 24.42 -162.76 -24.87 124.02 -143.97 114.20
USER
USER                  Rank         x       y       z       vdW    Elec       q     RMS
ATOM      1  N1  UDP     1      18.129  20.036  33.316    -0.34  -0.10  -0.211  2.112
ATOM      2  C2  UDP     1      18.455  21.346  33.100    -0.80  +0.27  +0.396  2.112
ATOM      3  N3  UDP     1      19.767  21.606  32.800    -0.53  -0.37  -0.440  2.112
ATOM      4  H3  UDP     1      20.024  22.592  32.651    +0.03  +0.61  +0.440  2.112
ATOM      5  C4  UDP     1      20.789  20.663  32.676    -0.70  +0.24  +0.396  2.112
ATOM      6  C5  UDP     1      20.382  19.312  32.907    -0.50  +0.00  +0.000  2.112
ATOM      7  C6  UDP     1      19.100  19.048  33.196    -0.45  +0.00  +0.000  2.112
ATOM      8  O2  UDP     1      17.618  22.247  33.185    -0.28  -0.32  -0.396  2.112
ATOM      9  O4  UDP     1      21.921  21.064  32.407    -0.19  -0.19  -0.396  2.112
ATOM     10  C1' UDP     1      16.743  19.689  33.659    -0.61  +0.07  +0.324  2.112
ATOM     11  C2' UDP     1      16.131  18.589  32.788    -0.64  -0.01  +0.113  2.112
ATOM     12  C3' UDP     1      15.014  18.078  33.728    -0.67  +0.00  +0.113  2.112
ATOM     13  C4' UDP     1      15.605  18.256  35.125    -0.53  +0.03  +0.113  2.112
```

```
ATOM     14  O4' UDP     1      16.789  19.080  34.943    -0.01  -0.08  -0.227  2.112
ATOM     15  O2' UDP     1      15.563  19.139  31.622    -0.29  +0.22  -0.537  2.112
ATOM     16  HO2'UDP     1      15.357  18.386  30.952    -0.19  -0.49  +0.424  2.112
ATOM     17  O3' UDP     1      13.895  18.955  33.563    -0.18  +0.07  -0.537  2.112
ATOM     18  HO3'UDP     1      14.220  19.862  33.198    -0.35  -0.37  +0.424  2.112
ATOM     19  C5' UDP     1      16.026  16.935  35.769    -0.36  +0.04  +0.113  2.112
ATOM     20  O5' UDP     1      16.746  17.237  36.949    +0.04  -0.15  -0.368  2.112
ATOM     21  PA  UDP     1      16.315  17.725  38.386    -0.63  +0.40  +1.019  2.112
ATOM     22  O1A UDP     1      17.557  17.965  39.176    -0.27  -0.04  -0.255  2.112
ATOM     23  O2A UDP     1      15.343  18.853  38.235    -0.10  -0.12  -0.255  2.112
ATOM     24  O3A UDP     1      15.653  16.343  38.828    -0.01  -0.22  -0.510  2.112
ATOM     25  PB  UDP     1      16.007  15.274  39.964    -0.67  +0.39  +1.019  2.112
ATOM     26  O1B UDP     1      15.929  16.105  41.347    -0.68  -0.26  -0.255  2.112
ATOM     27  O2B UDP     1      17.408  14.938  39.608    -0.02  -0.04  -0.255  2.112
ATOM     28  O3B UDP     1      14.997  14.197  40.130    -0.09  -0.10  -0.255  2.112
TER
ENDMDL
MODEL       98
USER    Run = 98
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.109 A
USER
USER    Estimated Free Energy of Binding    =   -7.94 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.51e-06     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -11.08 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.12 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.96 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.893783 19.279399 34.797086
USER    NEWDPF quat00.214303 0.443762 -0.870143 -7.171696
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-119.38 43.09 -179.96 146.93 -44.48 49.68 150.19
USER
USER                    Rank         x       y       z       vdW    Elec     q     RMS
ATOM      1  N1  UDP     1      18.342  20.174  33.229    -0.35  -0.10  -0.211  2.109
ATOM      2  C2  UDP     1      18.641  21.478  32.948    -0.82  +0.29  +0.396  2.109
ATOM      3  N3  UDP     1      19.966  21.769  32.746    -0.54  -0.38  -0.440  2.109
ATOM      4  H3  UDP     1      20.201  22.752  32.548    +0.03  +0.61  +0.440  2.109
ATOM      5  C4  UDP     1      21.026  20.862  32.782    -0.74  +0.25  +0.396  2.109
ATOM      6  C5  UDP     1      20.647  19.515  33.074    -0.53  +0.00  +0.000  2.109
ATOM      7  C6  UDP     1      19.353  19.220  33.267    -0.47  +0.00  +0.000  2.109
ATOM      8  O2  UDP     1      17.769  22.347  32.892    -0.28  -0.32  -0.396  2.109
ATOM      9  O4  UDP     1      22.164  21.290  32.585    -0.22  -0.20  -0.396  2.109
ATOM     10  C1' UDP     1      16.944  19.796  33.472    -0.63  +0.08  +0.324  2.109
ATOM     11  C2' UDP     1      16.451  18.614  32.634    -0.63  +0.00  +0.113  2.109
ATOM     12  C3' UDP     1      15.272  18.125  33.506    -0.65  -0.01  +0.113  2.109
ATOM     13  C4' UDP     1      15.727  18.423  34.933    -0.54  +0.03  +0.113  2.109
ATOM     14  O4' UDP     1      16.894  19.279  34.797    -0.02  -0.08  -0.227  2.109
ATOM     15  O2' UDP     1      15.973  19.058  31.386    -0.23  +0.16  -0.537  2.109
ATOM     16  HO2'UDP     1      14.967  18.852  31.309    -0.23  -0.38  +0.424  2.109
ATOM     17  O3' UDP     1      14.143  18.941  33.180    -0.24  +0.15  -0.537  2.109
ATOM     18  HO3'UDP     1      14.429  19.672  32.512    -0.27  -0.32  +0.424  2.109
ATOM     19  C5' UDP     1      16.133  17.168  35.707    -0.38  +0.04  +0.113  2.109
ATOM     20  O5' UDP     1      15.932  17.422  37.084    +0.05  -0.16  -0.368  2.109
ATOM     21  PA  UDP     1      16.853  18.005  38.224    -0.63  +0.36  +1.019  2.109
ATOM     22  O1A UDP     1      18.020  18.665  37.572    -0.11  -0.08  -0.255  2.109
ATOM     23  O2A UDP     1      16.007  18.819  39.152    -0.11  -0.11  -0.255  2.109
ATOM     24  O3A UDP     1      17.293  16.587  38.809    -0.11  -0.14  -0.510  2.109
ATOM     25  PB  UDP     1      16.529  15.472  39.664    -0.62  +0.35  +1.019  2.109
```

```
ATOM     26  O1B UDP     1      15.059  15.383  39.000    +0.05  -0.11  -0.255  2.109
ATOM     27  O2B UDP     1      16.487  16.122  40.998    -0.59  -0.22  -0.255  2.109
ATOM     28  O3B UDP     1      17.078  14.100  39.516    +0.06  -0.06  -0.255  2.109
TER
ENDMDL
MODEL       91
USER    Run = 91
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.427 A
USER
USER    Estimated Free Energy of Binding    =   -8.15 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.05e-06     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =   -11.05 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.33 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.72 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran017.439802 19.336859 35.113934
USER    NEWDPF quat0-0.853123 -0.282142 0.438836 8.841905
USER    NEWDPF ndihe7
USER    NEWDPF dihe0176.08 67.48 151.37 -55.37 -90.07 58.66 -174.00
USER
USER                    Rank         x       y       z       vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.914  19.999  33.457    -0.32  -0.12  -0.211  2.427
ATOM      2  C2  UDP     1      19.267  21.252  33.040    -0.78  +0.30  +0.396  2.427
ATOM      3  N3  UDP     1      20.601  21.462  32.804    -0.52  -0.33  -0.440  2.427
ATOM      4  H3  UDP     1      20.878  22.408  32.505    +0.03  +0.34  +0.440  2.427
ATOM      5  C4  UDP     1      21.621  20.517  32.931    -0.72  +0.26  +0.396  2.427
ATOM      6  C5  UDP     1      21.186  19.226  33.363    -0.49  +0.00  +0.000  2.427
ATOM      7  C6  UDP     1      19.882  19.010  33.590    -0.44  +0.00  +0.000  2.427
ATOM      8  O2  UDP     1      18.434  22.149  32.898    -0.26  -0.36  -0.396  2.427
ATOM      9  O4  UDP     1      22.775  20.871  32.687    -0.25  -0.27  -0.396  2.427
ATOM     10  C1' UDP     1      17.502  19.710  33.742    -0.57  +0.12  +0.324  2.427
ATOM     11  C2' UDP     1      16.951  18.471  33.033    -0.51  +0.01  +0.113  2.427
ATOM     12  C3' UDP     1      15.759  18.127  33.955    -0.54  +0.01  +0.113  2.427
ATOM     13  C4' UDP     1      16.238  18.552  35.342    -0.50  +0.04  +0.113  2.427
ATOM     14  O4' UDP     1      17.440  19.337  35.114    -0.02  -0.10  -0.227  2.427
ATOM     15  O2' UDP     1      16.483  18.804  31.747    -0.22  +0.08  -0.537  2.427
ATOM     16  HO2'UDP     1      16.132  17.957  31.279    -0.22  -0.27  +0.424  2.427
ATOM     17  O3' UDP     1      14.665  18.955  33.550    -0.16  +0.10  -0.537  2.427
ATOM     18  HO3'UDP     1      14.824  19.289  32.589    -0.09  -0.19  +0.424  2.427
ATOM     19  C5' UDP     1      16.595  17.367  36.241    -0.40  +0.05  +0.113  2.427
ATOM     20  O5' UDP     1      15.720  17.387  37.353    +0.13  -0.17  -0.368  2.427
ATOM     21  PA  UDP     1      15.712  18.191  38.710    -0.63  +0.44  +1.019  2.427
ATOM     22  O1A UDP     1      17.128  18.476  39.078    -0.17  -0.08  -0.255  2.427
ATOM     23  O2A UDP     1      14.768  19.345  38.575    -0.07  -0.12  -0.255  2.427
ATOM     24  O3A UDP     1      15.156  16.989  39.600    -0.15  -0.24  -0.510  2.427
ATOM     25  PB  UDP     1      15.860  15.759  40.340    -0.78  +0.49  +1.019  2.427
ATOM     26  O1B UDP     1      17.435  16.117  40.322    -0.47  -0.07  -0.255  2.427
ATOM     27  O2B UDP     1      15.543  14.649  39.405    -0.04  -0.11  -0.255  2.427
ATOM     28  O3B UDP     1      15.531  15.640  41.783    -0.74  -0.25  -0.255  2.427
TER
ENDMDL
MODEL       78
USER    Run = 78
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.417 A
USER
```

```
USER    Estimated Free Energy of Binding    =   -8.24 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +9.08e-07     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.97 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.42 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.55 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.577195 19.722656 34.915745
USER    NEWDPF quat0-0.672356 -0.299327 0.677009 17.193969
USER    NEWDPF ndihe7
USER    NEWDPF dihe0167.91 -111.85 -172.88 17.96 -34.07 -1.67 163.75
USER
USER                    Rank        x       y       z       vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.021  20.465  33.266   -0.40  -0.10  -0.211  2.417
ATOM      2  C2  UDP     1      18.220  21.723  32.770   -0.87  +0.27  +0.396  2.417
ATOM      3  N3  UDP     1      19.524  22.098  32.566   -0.51  -0.42  -0.440  2.417
ATOM      4  H3  UDP     1      19.683  23.050  32.207   +0.14  +0.59  +0.440  2.417
ATOM      5  C4  UDP     1      20.655  21.314  32.797   -0.77  +0.28  +0.396  2.417
ATOM      6  C5  UDP     1      20.378  20.008  33.308   -0.59  +0.00  +0.000  2.417
ATOM      7  C6  UDP     1      19.106  19.630  33.506   -0.51  +0.00  +0.000  2.417
ATOM      8  O2  UDP     1      17.281  22.485  32.533   -0.36  -0.26  -0.396  2.417
ATOM      9  O4  UDP     1      21.760  21.805  32.568   -0.08  -0.17  -0.396  2.417
ATOM     10  C1' UDP     1      16.650  20.006  33.523   -0.65  +0.06  +0.324  2.417
ATOM     11  C2' UDP     1      16.303  18.657  32.889   -0.62  +0.00  +0.113  2.417
ATOM     12  C3' UDP     1      15.127  18.217  33.792   -0.66  +0.00  +0.113  2.417
ATOM     13  C4' UDP     1      15.483  18.798  35.160   -0.56  +0.03  +0.113  2.417
ATOM     14  O4' UDP     1      16.577  19.723  34.916   -0.06  -0.07  -0.227  2.417
ATOM     15  O2' UDP     1      15.852  18.833  31.567   -0.24  +0.21  -0.537  2.417
ATOM     16  HO2'UDP     1      15.770  17.916  31.106   -0.31  -0.44  +0.424  2.417
ATOM     17  O3' UDP     1      13.951  18.856  33.289   -0.25  +0.10  -0.537  2.417
ATOM     18  HO3'UDP     1      13.234  18.888  34.027   -0.08  +0.11  +0.424  2.417
ATOM     19  C5' UDP     1      15.956  17.738  36.156   -0.39  +0.04  +0.113  2.417
ATOM     20  O5' UDP     1      15.393  18.045  37.417   +0.07  -0.17  -0.368  2.417
ATOM     21  PA  UDP     1      15.935  17.957  38.896   -0.71  +0.44  +1.019  2.417
ATOM     22  O1A UDP     1      17.421  18.066  38.841   -0.22  -0.06  -0.255  2.417
ATOM     23  O2A UDP     1      15.183  18.939  39.739   -0.23  -0.12  -0.255  2.417
ATOM     24  O3A UDP     1      15.514  16.436  39.126   -0.06  -0.22  -0.510  2.417
ATOM     25  PB  UDP     1      16.010  15.304  40.141   -0.69  +0.40  +1.019  2.417
ATOM     26  O1B UDP     1      15.993  16.019  41.590   -0.68  -0.30  -0.255  2.417
ATOM     27  O2B UDP     1      17.397  15.083  39.659   -0.06  -0.04  -0.255  2.417
ATOM     28  O3B UDP     1      15.076  14.159  40.290   -0.11  -0.11  -0.255  2.417
TER
ENDMDL
MODEL       67
USER    Run = 67
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.230 A
USER
USER    Estimated Free Energy of Binding    =   -8.10 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.15e-06     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.95 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.28 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.67 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
```

```
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran017.161973 19.546069 34.694746
USER    NEWDPF quat00.907012 0.421046 -0.007048 -17.600431
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-150.07 88.07 161.44 45.36 22.65 -28.61 139.40
USER
USER                    Rank        x       y       z       vdW    Elec      q     RMS
ATOM      1  N1  UDP     1       18.821  19.878  33.115    -0.32  -0.10  -0.211  2.230
ATOM      2  C2  UDP     1       19.295  21.037  32.566    -0.70  +0.25  +0.396  2.230
ATOM      3  N3  UDP     1       20.657  21.137  32.436    -0.49  -0.25  -0.440  2.230
ATOM      4  H3  UDP     1       21.023  22.012  32.037    -0.02  +0.11  +0.440  2.230
ATOM      5  C4  UDP     1       21.594  20.165  32.793    -0.67  +0.25  +0.396  2.230
ATOM      6  C5  UDP     1       21.034  18.976  33.354    -0.46  +0.00  +0.000  2.230
ATOM      7  C6  UDP     1       19.703  18.868  33.480    -0.43  +0.00  +0.000  2.230
ATOM      8  O2  UDP     1       18.542  21.948  32.218    -0.28  -0.26  -0.396  2.230
ATOM      9  O4  UDP     1       22.786  20.416  32.617    -0.21  -0.28  -0.396  2.230
ATOM     10  C1' UDP     1       17.373  19.713  33.298    -0.61  +0.10  +0.324  2.230
ATOM     11  C2' UDP     1       16.804  18.416  32.716    -0.56  +0.00  +0.113  2.230
ATOM     12  C3' UDP     1       15.512  18.276  33.555    -0.62  +0.00  +0.113  2.230
ATOM     13  C4' UDP     1       15.894  18.870  34.910    -0.55  +0.02  +0.113  2.230
ATOM     14  O4' UDP     1       17.162  19.546  34.695    -0.04  -0.09  -0.227  2.230
ATOM     15  O2' UDP     1       16.478  18.585  31.357    -0.23  +0.12  -0.537  2.230
ATOM     16  HO2'UDP     1       15.659  18.004  31.125    -0.34  -0.45  +0.424  2.230
ATOM     17  O3' UDP     1       14.519  19.096  32.932    -0.11  +0.21  -0.537  2.230
ATOM     18  HO3'UDP     1       14.585  18.999  31.909    -0.17  -0.30  +0.424  2.230
ATOM     19  C5' UDP     1       16.086  17.810  35.995    -0.44  +0.04  +0.113  2.230
ATOM     20  O5' UDP     1       16.063  18.464  37.250    -0.05  -0.16  -0.368  2.230
ATOM     21  PA  UDP     1       16.420  18.005  38.717    -0.68  +0.39  +1.019  2.230
ATOM     22  O1A UDP     1       17.896  18.128  38.884    -0.25  -0.03  -0.255  2.230
ATOM     23  O2A UDP     1       15.535  18.739  39.674    -0.21  -0.12  -0.255  2.230
ATOM     24  O3A UDP     1       16.027  16.474  38.501    +0.00  -0.22  -0.510  2.230
ATOM     25  PB  UDP     1       15.939  15.218  39.486    -0.59  +0.40  +1.019  2.230
ATOM     26  O1B UDP     1       15.737  15.862  40.954    -0.53  -0.17  -0.255  2.230
ATOM     27  O2B UDP     1       17.298  14.640  39.327    -0.02  -0.06  -0.255  2.230
ATOM     28  O3B UDP     1       14.736  14.368  39.294    -0.02  -0.11  -0.255  2.230
TER
ENDMDL
MODEL        4
USER    Run = 4
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.180 A
USER
USER    Estimated Free Energy of Binding    =   -7.94 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.52e-06      [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.90 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.12 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.79 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.815113 19.444013 34.902784
USER    NEWDPF quat0-0.630271 -0.262187 0.730764 9.610976
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-171.96 113.05 85.63 129.04 -22.39 18.54 152.66
USER
USER                    Rank        x       y       z       vdW    Elec      q     RMS
ATOM      1  N1  UDP     1       18.242  20.226  33.257    -0.36  -0.10  -0.211  2.180
ATOM      2  C2  UDP     1       18.524  21.507  32.871    -0.82  +0.28  +0.396  2.180
ATOM      3  N3  UDP     1       19.844  21.797  32.636    -0.54  -0.37  -0.440  2.180
ATOM      4  H3  UDP     1       20.066  22.763  32.359    +0.06  +0.53  +0.440  2.180
ATOM      5  C4  UDP     1       20.915  20.907  32.736    -0.74  +0.25  +0.396  2.180
```

```
ATOM      6  C5  UDP     1      20.553  19.584  33.137    -0.54  +0.00  +0.000  2.180
ATOM      7  C6  UDP     1      19.264  19.290  33.364    -0.47  +0.00  +0.000  2.180
ATOM      8  O2  UDP     1      17.642  22.360  32.753    -0.31  -0.30  -0.396  2.180
ATOM      9  O4  UDP     1      22.046  21.330  32.496    -0.20  -0.18  -0.396  2.180
ATOM     10  C1' UDP     1      16.850  19.854  33.541    -0.64  +0.07  +0.324  2.180
ATOM     11  C2' UDP     1      16.365  18.604  32.803    -0.62  +0.00  +0.113  2.180
ATOM     12  C3' UDP     1      15.198  18.172  33.720    -0.65  +0.00  +0.113  2.180
ATOM     13  C4' UDP     1      15.660  18.589  35.116    -0.55  +0.03  +0.113  2.180
ATOM     14  O4' UDP     1      16.815  19.444  34.903    -0.04  -0.08  -0.227  2.180
ATOM     15  O2' UDP     1      15.874  18.941  31.527    -0.25  +0.19  -0.537  2.180
ATOM     16  HO2'UDP     1      15.387  18.131  31.120    -0.23  -0.51  +0.424  2.180
ATOM     17  O3' UDP     1      14.058  18.948  33.339    -0.21  +0.12  -0.537  2.180
ATOM     18  HO3'UDP     1      13.771  18.691  32.384    -0.14  -0.17  +0.424  2.180
ATOM     19  C5' UDP     1      16.085  17.404  35.983    -0.40  +0.04  +0.113  2.180
ATOM     20  O5' UDP     1      15.837  17.743  37.334    +0.02  -0.16  -0.368  2.180
ATOM     21  PA  UDP     1      16.755  17.840  38.614    -0.68  +0.36  +1.019  2.180
ATOM     22  O1A UDP     1      18.070  18.398  38.187    -0.18  -0.04  -0.255  2.180
ATOM     23  O2A UDP     1      15.999  18.554  39.690    -0.10  -0.12  -0.255  2.180
ATOM     24  O3A UDP     1      16.882  16.265  38.834    -0.06  -0.17  -0.510  2.180
ATOM     25  PB  UDP     1      16.028  15.206  39.673    -0.62  +0.38  +1.019  2.180
ATOM     26  O1B UDP     1      15.954  15.827  41.162    -0.61  -0.20  -0.255  2.180
ATOM     27  O2B UDP     1      16.921  14.021  39.621    +0.04  -0.06  -0.255  2.180
ATOM     28  O3B UDP     1      14.607  15.093  39.256    +0.05  -0.09  -0.255  2.180
TER
ENDMDL
MODEL       68
USER    Run = 68
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.052 A
USER
USER    Estimated Free Energy of Binding    =   -8.04 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.27e-06     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.89 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.22 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.67 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran017.046913 18.963031 34.725298
USER    NEWDPF quat0-0.538364 0.625258 -0.564993 -1.207985
USER    NEWDPF ndihe7
USER    NEWDPF dihe0177.60 43.09 -156.33 -38.18 133.10 -146.64 118.61
USER
USER                    Rank        x       y       z       vdW    Elec       q     RMS
ATOM      1  N1  UDP     1      18.510  19.778  33.128    -0.31  -0.10  -0.211  2.052
ATOM      2  C2  UDP     1      18.922  21.058  32.881    -0.73  +0.26  +0.396  2.052
ATOM      3  N3  UDP     1      20.259  21.229  32.630    -0.50  -0.29  -0.440  2.052
ATOM      4  H3  UDP     1      20.580  22.192  32.458    +0.03  +0.34  +0.440  2.052
ATOM      5  C4  UDP     1      21.227  20.224  32.585    -0.66  +0.23  +0.396  2.052
ATOM      6  C5  UDP     1      20.731  18.909  32.845    -0.47  +0.00  +0.000  2.052
ATOM      7  C6  UDP     1      19.424  18.731  33.086    -0.43  +0.00  +0.000  2.052
ATOM      8  O2  UDP     1      18.137  22.008  32.896    -0.26  -0.31  -0.396  2.052
ATOM      9  O4  UDP     1      22.391  20.549  32.353    -0.22  -0.24  -0.396  2.052
ATOM     10  C1' UDP     1      17.093  19.525  33.419    -0.59  +0.08  +0.324  2.052
ATOM     11  C2' UDP     1      16.453  18.431  32.561    -0.62  -0.01  +0.113  2.052
ATOM     12  C3' UDP     1      15.268  18.022  33.467    -0.64  -0.01  +0.113  2.052
ATOM     13  C4' UDP     1      15.809  18.217  34.883    -0.51  +0.03  +0.113  2.052
ATOM     14  O4' UDP     1      17.047  18.963  34.725    +0.01  -0.08  -0.227  2.052
ATOM     15  O2' UDP     1      15.969  18.969  31.353    -0.23  +0.17  -0.537  2.052
ATOM     16  HO2'UDP     1      15.535  18.222  30.793    -0.25  -0.50  +0.424  2.052
ATOM     17  O3' UDP     1      14.212  18.955  33.222    -0.23  +0.14  -0.537  2.052
```

```
ATOM     18  HO3'UDP     1      14.540  19.681  32.569    -0.27  -0.29  +0.424  2.052
ATOM     19  C5' UDP     1      16.123  16.899  35.591    -0.36  +0.04  +0.113  2.052
ATOM     20  O5' UDP     1      16.716  17.206  36.838    +0.04  -0.15  -0.368  2.052
ATOM     21  PA  UDP     1      16.152  17.782  38.194    -0.58  +0.41  +1.019  2.052
ATOM     22  O1A UDP     1      17.314  18.186  39.035    -0.21  -0.07  -0.255  2.052
ATOM     23  O2A UDP     1      15.113  18.813  37.878    -0.06  -0.12  -0.255  2.052
ATOM     24  O3A UDP     1      15.562  16.395  38.718    +0.02  -0.22  -0.510  2.052
ATOM     25  PB  UDP     1      16.071  15.327  39.793    -0.64  +0.39  +1.019  2.052
ATOM     26  O1B UDP     1      16.010  16.107  41.207    -0.68  -0.24  -0.255  2.052
ATOM     27  O2B UDP     1      17.471  15.121  39.345    -0.08  -0.05  -0.255  2.052
ATOM     28  O3B UDP     1      15.166  14.165  39.982    -0.08  -0.11  -0.255  2.052
TER
ENDMDL
MODEL        69
USER    Run = 69
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.378 A
USER
USER    Estimated Free Energy of Binding    =   -8.23 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +9.27e-07      [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.89 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.41 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.48 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.201952 19.564603 34.695888
USER    NEWDPF quat00.514657 0.516195 -0.684595 -28.099016
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-150.93 172.72 28.50 65.97 16.78 -26.91 120.36
USER
USER                 Rank     x       y       z      vdW    Elec     q     RMS
ATOM      1  N1  UDP     1      17.763  20.463  33.243    -0.42  -0.09  -0.211  2.378
ATOM      2  C2  UDP     1      17.856  21.722  32.717    -0.89  +0.25  +0.396  2.378
ATOM      3  N3  UDP     1      19.109  22.280  32.690    -0.54  -0.45  -0.440  2.378
ATOM      4  H3  UDP     1      19.185  23.233  32.309    +0.08  +0.65  +0.440  2.378
ATOM      5  C4  UDP     1      20.290  21.679  33.128    -0.78  +0.38  +0.396  2.378
ATOM      6  C5  UDP     1      20.126  20.363  33.660    -0.64  +0.00  +0.000  2.378
ATOM      7  C6  UDP     1      18.906  19.807  33.686    -0.53  +0.00  +0.000  2.378
ATOM      8  O2  UDP     1      16.866  22.328  32.302    -0.32  -0.21  -0.396  2.378
ATOM      9  O4  UDP     1      21.336  22.322  33.040    -0.42  -0.38  -0.396  2.378
ATOM     10  C1' UDP     1      16.448  19.813  33.317    -0.66  +0.03  +0.324  2.378
ATOM     11  C2' UDP     1      16.399  18.409  32.710    -0.60  -0.01  +0.113  2.378
ATOM     12  C3' UDP     1      15.173  17.827  33.450    -0.64  -0.01  +0.113  2.378
ATOM     13  C4' UDP     1      15.226  18.495  34.823    -0.59  +0.02  +0.113  2.378
ATOM     14  O4' UDP     1      16.202  19.565  34.696    -0.06  -0.05  -0.227  2.378
ATOM     15  O2' UDP     1      16.139  18.476  31.327    -0.19  +0.22  -0.537  2.378
ATOM     16  HO2'UDP     1      15.599  17.649  31.039    -0.17  -0.64  +0.424  2.378
ATOM     17  O3' UDP     1      14.010  18.269  32.744    -0.37  +0.13  -0.537  2.378
ATOM     18  HO3'UDP     1      13.434  17.455  32.486    -0.01  +0.09  +0.424  2.378
ATOM     19  C5' UDP     1      15.684  17.548  35.932    -0.25  +0.04  +0.113  2.378
ATOM     20  O5' UDP     1      15.763  18.291  37.133    -0.03  -0.16  -0.368  2.378
ATOM     21  PA  UDP     1      16.398  18.000  38.548    -0.66  +0.40  +1.019  2.378
ATOM     22  O1A UDP     1      17.873  18.184  38.429    -0.21  -0.04  -0.255  2.378
ATOM     23  O2A UDP     1      15.664  18.804  39.575    -0.15  -0.12  -0.255  2.378
ATOM     24  O3A UDP     1      16.048  16.444  38.559    -0.01  -0.21  -0.510  2.378
ATOM     25  PB  UDP     1      15.798  15.387  39.732    -0.65  +0.40  +1.019  2.378
ATOM     26  O1B UDP     1      17.089  14.416  39.690    +0.06  -0.05  -0.255  2.378
ATOM     27  O2B UDP     1      14.581  14.697  39.235    -0.01  -0.10  -0.255  2.378
ATOM     28  O3B UDP     1      15.825  15.967  41.099    -0.63  -0.20  -0.255  2.378
TER
```

```
ENDMDL
MODEL        61
USER    Run = 61
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.557 A
USER
USER    Estimated Free Energy of Binding    =   -7.87 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.71e-06      [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.89 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.05 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.84 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.562668 19.480276 35.364105
USER    NEWDPF quat00.504391 0.164975 -0.847569 -18.647284
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-178.72 70.98 -178.92 -84.93 -87.09 46.14 171.15
USER
USER                    Rank         x       y       z       vdW    Elec       q     RMS
ATOM      1  N1  UDP     1       17.871  20.369  33.675    -0.39  -0.10  -0.211  2.557
ATOM      2  C2  UDP     1       17.960  21.651  33.210    -0.86  +0.28  +0.396  2.557
ATOM      3  N3  UDP     1       19.223  22.123  32.959    -0.53  -0.48  -0.440  2.557
ATOM      4  H3  UDP     1       19.299  23.093  32.623    +0.05  +0.79  +0.440  2.557
ATOM      5  C4  UDP     1       20.415  21.414  33.114    -0.78  +0.34  +0.396  2.557
ATOM      6  C5  UDP     1       20.254  20.078  33.596    -0.59  +0.00  +0.000  2.557
ATOM      7  C6  UDP     1       19.022  19.606  33.839    -0.51  +0.00  +0.000  2.557
ATOM      8  O2  UDP     1       16.960  22.352  33.040    -0.29  -0.28  -0.396  2.557
ATOM      9  O4  UDP     1       21.471  21.988  32.850    -0.19  -0.27  -0.396  2.557
ATOM     10  C1' UDP     1       16.549  19.807  33.979    -0.60  +0.06  +0.324  2.557
ATOM     11  C2' UDP     1       16.266  18.455  33.319    -0.55  +0.00  +0.113  2.557
ATOM     12  C3' UDP     1       15.168  17.908  34.261    -0.59  +0.01  +0.113  2.557
ATOM     13  C4' UDP     1       15.548  18.474  35.629    -0.53  +0.04  +0.113  2.557
ATOM     14  O4' UDP     1       16.563  19.480  35.364    -0.04  -0.08  -0.227  2.557
ATOM     15  O2' UDP     1       15.742  18.636  32.025    -0.22  +0.20  -0.537  2.557
ATOM     16  HO2'UDP     1       15.492  17.722  31.624    -0.22  -0.46  +0.424  2.557
ATOM     17  O3' UDP     1       13.928  18.477  33.832    -0.23  -0.03  -0.537  2.557
ATOM     18  HO3'UDP     1       13.998  18.747  32.840    -0.09  -0.13  +0.424  2.557
ATOM     19  C5' UDP     1       16.139  17.422  36.568    -0.38  +0.05  +0.113  2.557
ATOM     20  O5' UDP     1       15.490  17.543  37.819    +0.16  -0.17  -0.368  2.557
ATOM     21  PA  UDP     1       15.833  18.324  39.146    -0.55  +0.45  +1.019  2.557
ATOM     22  O1A UDP     1       17.314  18.480  39.212    -0.19  -0.07  -0.255  2.557
ATOM     23  O2A UDP     1       14.987  19.558  39.205    -0.14  -0.10  -0.255  2.557
ATOM     24  O3A UDP     1       15.367  17.162  40.135    -0.28  -0.28  -0.510  2.557
ATOM     25  PB  UDP     1       15.773  15.623  40.282    -0.75  +0.45  +1.019  2.557
ATOM     26  O1B UDP     1       17.381  15.607  40.125    -0.17  -0.04  -0.255  2.557
ATOM     27  O2B UDP     1       15.104  15.041  39.091    -0.01  -0.11  -0.255  2.557
ATOM     28  O3B UDP     1       15.535  15.049  41.631    -0.49  -0.17  -0.255  2.557
TER
ENDMDL
MODEL        6
USER    Run = 6
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.174 A
USER
USER    Estimated Free Energy of Binding    =   -8.10 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.16e-06      [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.88 kcal/mol  [=(1)+(2)]
```

```
USER
USER    (1) Final Intermolecular Energy     =  -10.28 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.60 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.843938 19.665299 34.549841
USER    NEWDPF quat0-0.680946 -0.646119 0.344735 19.606725
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-164.02 79.05 -46.01 2.37 80.35 -64.66 114.70
USER
USER                    Rank        x       y       z       vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.554  20.272  33.114    -0.36  -0.11  -0.211  2.174
ATOM      2  C2  UDP     1      18.912  21.504  32.639    -0.81  +0.28  +0.396  2.174
ATOM      3  N3  UDP     1      20.255  21.782  32.618    -0.53  -0.35  -0.440  2.174
ATOM      4  H3  UDP     1      20.531  22.713  32.276    +0.10  +0.38  +0.440  2.174
ATOM      5  C4  UDP     1      21.282  20.924  33.014    -0.75  +0.28  +0.396  2.174
ATOM      6  C5  UDP     1      20.843  19.651  33.492    -0.54  +0.00  +0.000  2.174
ATOM      7  C6  UDP     1      19.532  19.368  33.512    -0.48  +0.00  +0.000  2.174
ATOM      8  O2  UDP     1      18.073  22.325  32.265    -0.33  -0.27  -0.396  2.174
ATOM      9  O4  UDP     1      22.441  21.332  32.938    -0.25  -0.27  -0.396  2.174
ATOM     10  C1' UDP     1      17.131  19.916  33.179    -0.66  +0.08  +0.324  2.174
ATOM     11  C2' UDP     1      16.779  18.583  32.514    -0.61  +0.00  +0.113  2.174
ATOM     12  C3' UDP     1      15.460  18.244  33.247    -0.64  -0.01  +0.113  2.174
ATOM     13  C4' UDP     1      15.662  18.825  34.646    -0.57  +0.02  +0.113  2.174
ATOM     14  O4' UDP     1      16.844  19.665  34.550    -0.06  -0.07  -0.227  2.174
ATOM     15  O2' UDP     1      16.532  18.765  31.140    -0.20  +0.10  -0.537  2.174
ATOM     16  HO2'UDP     1      16.002  17.960  30.776    -0.43  -0.37  +0.424  2.174
ATOM     17  O3' UDP     1      14.416  18.955  32.577    -0.24  +0.24  -0.537  2.174
ATOM     18  HO3'UDP     1      14.645  19.040  31.576    -0.24  -0.35  +0.424  2.174
ATOM     19  C5' UDP     1      15.913  17.753  35.708    -0.43  +0.04  +0.113  2.174
ATOM     20  O5' UDP     1      16.283  18.408  36.906    -0.03  -0.15  -0.368  2.174
ATOM     21  PA  UDP     1      16.194  18.010  38.430    -0.64  +0.41  +1.019  2.174
ATOM     22  O1A UDP     1      17.443  18.479  39.096    -0.19  -0.06  -0.255  2.174
ATOM     23  O2A UDP     1      14.882  18.484  38.971    -0.19  -0.12  -0.255  2.174
ATOM     24  O3A UDP     1      16.272  16.435  38.184    +0.02  -0.21  -0.510  2.174
ATOM     25  PB  UDP     1      16.972  15.237  38.979    -0.52  +0.35  +1.019  2.174
ATOM     26  O1B UDP     1      16.522  13.903  38.187    +0.08  -0.16  -0.255  2.174
ATOM     27  O2B UDP     1      16.297  15.342  40.297    -0.20  -0.09  -0.255  2.174
ATOM     28  O3B UDP     1      18.455  15.227  38.895    -0.11  -0.04  -0.255  2.174
TER
ENDMDL
MODEL       26
USER    Run = 26
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.271 A
USER
USER    Estimated Free Energy of Binding    =   -8.13 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.09e-06     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.83 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.31 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.51 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.632623 19.448723 35.340054
USER    NEWDPF quat00.615270 -0.245958 -0.748964 -10.093568
USER    NEWDPF ndihe7
```

```
USER    NEWDPF dihe0174.97 44.52 29.30 28.43 75.61 -90.02 127.13
USER
USER                    Rank      x       y       z      vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      17.907  20.223  33.570   -0.37  -0.10  -0.211  2.271
ATOM      2  C2  UDP     1      18.147  21.502  33.150   -0.83  +0.27  +0.396  2.271
ATOM      3  N3  UDP     1      19.440  21.795  32.799   -0.55  -0.39  -0.440  2.271
ATOM      4  H3  UDP     1      19.633  22.760  32.496   +0.03  +0.60  +0.440  2.271
ATOM      5  C4  UDP     1      20.521  20.911  32.812   -0.73  +0.26  +0.396  2.271
ATOM      6  C5  UDP     1      20.202  19.590  33.254   -0.53  +0.00  +0.000  2.271
ATOM      7  C6  UDP     1      18.939  19.292  33.595   -0.47  +0.00  +0.000  2.271
ATOM      8  O2  UDP     1      17.254  22.350  33.103   -0.29  -0.30  -0.396  2.271
ATOM      9  O4  UDP     1      21.624  21.337  32.472   -0.20  -0.19  -0.396  2.271
ATOM     10  C1' UDP     1      16.547  19.847  33.977   -0.61  +0.06  +0.324  2.271
ATOM     11  C2' UDP     1      16.006  18.589  33.294   -0.60  +0.00  +0.113  2.271
ATOM     12  C3' UDP     1      14.925  18.160  34.313   -0.62  +0.01  +0.113  2.271
ATOM     13  C4' UDP     1      15.505  18.590  35.660   -0.52  +0.04  +0.113  2.271
ATOM     14  O4' UDP     1      16.633  19.449  35.340   -0.04  -0.09  -0.227  2.271
ATOM     15  O2' UDP     1      15.403  18.914  32.063   -0.26  +0.22  -0.537  2.271
ATOM     16  HO2'UDP     1      15.076  18.053  31.602   -0.18  -0.46  +0.424  2.271
ATOM     17  O3' UDP     1      13.752  18.927  34.026   -0.09  -0.03  -0.537  2.271
ATOM     18  HO3'UDP     1      13.950  19.584  33.258   -0.37  -0.26  +0.424  2.271
ATOM     19  C5' UDP     1      16.010  17.414  36.496   -0.36  +0.05  +0.113  2.271
ATOM     20  O5' UDP     1      16.440  17.923  37.745   -0.05  -0.15  -0.368  2.271
ATOM     21  PA  UDP     1      16.141  17.518  39.240   -0.77  +0.43  +1.019  2.271
ATOM     22  O1A UDP     1      17.435  17.530  39.981   -0.35  -0.07  -0.255  2.271
ATOM     23  O2A UDP     1      15.025  18.373  39.752   -0.26  -0.13  -0.255  2.271
ATOM     24  O3A UDP     1      15.720  16.014  38.913   -0.02  -0.22  -0.510  2.271
ATOM     25  PB  UDP     1      15.458  14.728  39.827   -0.57  +0.39  +1.019  2.271
ATOM     26  O1B UDP     1      16.713  13.754  39.531   +0.02  -0.08  -0.255  2.271
ATOM     27  O2B UDP     1      14.207  14.205  39.222   -0.02  -0.10  -0.255  2.271
ATOM     28  O3B UDP     1      15.535  14.985  41.287   -0.38  -0.14  -0.255  2.271
TER
ENDMDL
MODEL       44
USER    Run = 44
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.334 A
USER
USER    Estimated Free Energy of Binding    =   -8.06 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.24e-06     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.79 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -10.24 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.55 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.271561 19.593224 34.779030
USER    NEWDPF quat00.519881 0.500873 -0.691990 -26.382845
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-7.19 74.61 -113.35 69.18 12.29 -18.57 135.17
USER
USER                    Rank      x       y       z      vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      17.817  20.480  33.302   -0.41  -0.10  -0.211  2.334
ATOM      2  C2  UDP     1      17.921  21.743  32.788   -0.89  +0.26  +0.396  2.334
ATOM      3  N3  UDP     1      19.183  22.278  32.739   -0.53  -0.47  -0.440  2.334
ATOM      4  H3  UDP     1      19.268  23.234  32.368   +0.08  +0.70  +0.440  2.334
ATOM      5  C4  UDP     1      20.363  21.651  33.144   -0.77  +0.38  +0.396  2.334
ATOM      6  C5  UDP     1      20.186  20.332  33.665   -0.63  +0.00  +0.000  2.334
ATOM      7  C6  UDP     1      18.957  19.798  33.711   -0.53  +0.00  +0.000  2.334
ATOM      8  O2  UDP     1      16.934  22.372  32.403   -0.35  -0.22  -0.396  2.334
ATOM      9  O4  UDP     1      21.418  22.276  33.040   -0.41  -0.36  -0.396  2.334
```

```
ATOM     10  C1' UDP     1      16.492  19.853  33.398   -0.66  +0.04  +0.324  2.334
ATOM     11  C2' UDP     1      16.403  18.458  32.776   -0.60  +0.00  +0.113  2.334
ATOM     12  C3' UDP     1      15.183  17.889  33.537   -0.65  -0.01  +0.113  2.334
ATOM     13  C4' UDP     1      15.279  18.540  34.916   -0.58  +0.02  +0.113  2.334
ATOM     14  O4' UDP     1      16.272  19.593  34.779   -0.06  -0.05  -0.227  2.334
ATOM     15  O2' UDP     1      16.113  18.546  31.401   -0.21  +0.21  -0.537  2.334
ATOM     16 HO2'UDP     1      15.957  19.531  31.145   -0.05  -0.08  +0.424  2.334
ATOM     17  O3' UDP     1      14.013  18.361  32.862   -0.36  +0.11  -0.537  2.334
ATOM     18 HO3'UDP     1      14.233  18.530  31.870   -0.10  -0.32  +0.424  2.334
ATOM     19  C5' UDP     1      15.744  17.572  36.003   -0.24  +0.04  +0.113  2.334
ATOM     20  O5' UDP     1      15.535  18.194  37.257   -0.02  -0.17  -0.368  2.334
ATOM     21  PA  UDP     1      16.149  17.970  38.693   -0.69  +0.42  +1.019  2.334
ATOM     22  O1A UDP     1      17.550  18.480  38.673   -0.16  -0.06  -0.255  2.334
ATOM     23  O2A UDP     1      15.204  18.533  39.708   -0.25  -0.12  -0.255  2.334
ATOM     24  O3A UDP     1      16.154  16.376  38.613   -0.01  -0.21  -0.510  2.334
ATOM     25  PB  UDP     1      16.024  15.225  39.715   -0.63  +0.39  +1.019  2.334
ATOM     26  O1B UDP     1      14.558  14.590  39.472   +0.02  -0.09  -0.255  2.334
ATOM     27  O2B UDP     1      16.070  16.026  40.965   -0.59  -0.20  -0.255  2.334
ATOM     28  O3B UDP     1      16.951  14.082  39.523   +0.03  -0.07  -0.255  2.334
TER
ENDMDL
MODEL       93
USER    Run = 93
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.047 A
USER
USER    Estimated Free Energy of Binding    =   -7.80 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +1.91e-06      [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.78 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =   -9.98 kcal/mol
USER    (2) Final_Internal Energy of Ligand =   -0.80 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran017.106934 19.121410 34.610553
USER    NEWDPF quat00.289729 0.319963 -0.902043 -3.357918
USER    NEWDPF ndihe7
USER    NEWDPF dihe0169.72 84.68 85.45 74.96 138.36 -122.86 108.33
USER
USER                    Rank       x       y       z      vdW     Elec       q     RMS
ATOM      1  N1  UDP     1      18.546  19.949  32.998   -0.33  -0.10  -0.211  2.047
ATOM      2  C2  UDP     1      18.907  21.237  32.717   -0.76  +0.26  +0.396  2.047
ATOM      3  N3  UDP     1      20.238  21.457  32.468   -0.51  -0.29  -0.440  2.047
ATOM      4  H3  UDP     1      20.521  22.426  32.271   +0.06  +0.32  +0.440  2.047
ATOM      5  C4  UDP     1      21.246  20.491  32.458   -0.69  +0.22  +0.396  2.047
ATOM      6  C5  UDP     1      20.802  19.165  32.752   -0.50  +0.00  +0.000  2.047
ATOM      7  C6  UDP     1      19.502  18.940  32.991   -0.45  +0.00  +0.000  2.047
ATOM      8  O2  UDP     1      18.085  22.155  32.701   -0.29  -0.30  -0.396  2.047
ATOM      9  O4  UDP     1      22.398  20.856  32.223   -0.24  -0.20  -0.396  2.047
ATOM     10  C1' UDP     1      17.138  19.648  33.289   -0.62  +0.08  +0.324  2.047
ATOM     11  C2' UDP     1      16.549  18.505  32.459   -0.63  -0.01  +0.113  2.047
ATOM     12  C3' UDP     1      15.376  18.073  33.370   -0.63  -0.01  +0.113  2.047
ATOM     13  C4' UDP     1      15.900  18.331  34.782   -0.51  +0.02  +0.113  2.047
ATOM     14  O4' UDP     1      17.107  19.121  34.611   +0.00  -0.08  -0.227  2.047
ATOM     15  O2' UDP     1      16.052  18.988  31.233   -0.22  +0.16  -0.537  2.047
ATOM     16 HO2'UDP     1      15.773  18.195  30.639   -0.30  -0.42  +0.424  2.047
ATOM     17  O3' UDP     1      14.285  18.955  33.093   -0.25  +0.16  -0.537  2.047
ATOM     18 HO3'UDP     1      14.263  19.168  32.085   -0.19  -0.31  +0.424  2.047
ATOM     19  C5' UDP     1      16.262  17.047  35.530   -0.36  +0.04  +0.113  2.047
ATOM     20  O5' UDP     1      17.045  17.404  36.653   +0.03  -0.15  -0.368  2.047
ATOM     21  PA  UDP     1      16.709  17.643  38.176   -0.62  +0.37  +1.019  2.047
```

```
ATOM     22  O1A UDP     1      17.832  18.422  38.771    -0.20  -0.04  -0.255  2.047
ATOM     23  O2A UDP     1      15.325  18.205  38.276    -0.06  -0.12  -0.255  2.047
ATOM     24  O3A UDP     1      16.828  16.111  38.604    -0.03  -0.18  -0.510  2.047
ATOM     25  PB  UDP     1      16.043  15.207  39.663    -0.62  +0.38  +1.019  2.047
ATOM     26  O1B UDP     1      16.135  16.029  41.051    -0.62  -0.21  -0.255  2.047
ATOM     27  O2B UDP     1      16.902  13.995  39.690    +0.04  -0.06  -0.255  2.047
ATOM     28  O3B UDP     1      14.585  15.087  39.409    +0.08  -0.08  -0.255  2.047
TER
ENDMDL
MODEL       16
USER    Run = 16
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 1.845 A
USER
USER    Estimated Free Energy of Binding    =   -7.59 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +2.73e-06      [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.63 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =   -9.77 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.86 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.760984 19.372334 34.613037
USER    NEWDPF quat00.476570 0.558632 -0.678831 -I0.358588
USER    NEWDPF ndihe7
USER    NEWDPF dihe0-179.67 65.79 64.64 -43.11 -39.67 2.21 151.27
USER
USER                    Rank         x       y       z      vdW     Elec       q     RMS
ATOM      1  N1  UDP     1      18.274  20.197  33.068    -0.36  -0.10  -0.211  1.845
ATOM      2  C2  UDP     1      18.571  21.487  32.727    -0.82  +0.27  +0.396  1.845
ATOM      3  N3  UDP     1      19.901  21.786  32.572    -0.54  -0.35  -0.440  1.845
ATOM      4  H3  UDP     1      20.134  22.759  32.330    +0.06  +0.51  +0.440  1.845
ATOM      5  C4  UDP     1      20.968  20.897  32.711    -0.74  +0.24  +0.396  1.845
ATOM      6  C5  UDP     1      20.591  19.564  33.061    -0.54  +0.00  +0.000  1.845
ATOM      7  C6  UDP     1      19.293  19.261  33.209    -0.47  +0.00  +0.000  1.845
ATOM      8  O2  UDP     1      17.693  22.340  32.580    -0.33  -0.28  -0.396  1.845
ATOM      9  O4  UDP     1      22.109  21.329  32.545    -0.21  -0.19  -0.396  1.845
ATOM     10  C1' UDP     1      16.870  19.813  33.265    -0.66  +0.07  +0.324  1.845
ATOM     11  C2' UDP     1      16.432  18.579  32.473    -0.65  -0.01  +0.113  1.845
ATOM     12  C3' UDP     1      15.217  18.123  33.314    -0.67  -0.02  +0.113  1.845
ATOM     13  C4' UDP     1      15.599  18.509  34.742    -0.56  +0.02  +0.113  1.845
ATOM     14  O4' UDP     1      16.761  19.372  34.613    -0.03  -0.07  -0.227  1.845
ATOM     15  O2' UDP     1      16.010  18.945  31.180    -0.23  +0.17  -0.537  1.845
ATOM     16  HO2'UDP     1      15.668  18.111  30.681    -0.27  -0.50  +0.424  1.845
ATOM     17  O3' UDP     1      14.097  18.904  32.887    -0.25  +0.19  -0.537  1.845
ATOM     18  HO3'UDP     1      14.295  19.315  31.964    -0.22  -0.35  +0.424  1.845
ATOM     19  C5' UDP     1      15.981  17.305  35.605    -0.39  +0.04  +0.113  1.845
ATOM     20  O5' UDP     1      15.686  17.625  36.951    +0.07  -0.16  -0.368  1.845
ATOM     21  PA  UDP     1      16.448  17.389  38.312    -0.60  +0.39  +1.019  1.845
ATOM     22  O1A UDP     1      17.886  17.155  37.993    -0.10  -0.06  -0.255  1.845
ATOM     23  O2A UDP     1      16.103  18.502  39.251    -0.18  -0.11  -0.255  1.845
ATOM     24  O3A UDP     1      15.738  16.001  38.649    +0.03  -0.22  -0.510  1.845
ATOM     25  PB  UDP     1      16.164  14.475  38.440    -0.39  +0.54  +1.019  1.845
ATOM     26  O1B UDP     1      16.007  14.220  36.852    -0.22  -0.29  -0.255  1.845
ATOM     27  O2B UDP     1      15.104  13.778  39.211    +0.01  -0.13  -0.255  1.845
ATOM     28  O3B UDP     1      17.597  14.193  38.713    +0.00  -0.10  -0.255  1.845
TER
ENDMDL
MODEL       15
USER    Run = 15
USER    Cluster Rank = 1
```

```
USER    Number of conformations in this cluster = 30
USER
USER    RMSD from reference structure       = 2.223 A
USER
USER    Estimated Free Energy of Binding    =   -7.66 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +2.43e-06     [Temperature = 298.15 K]
USER
USER    Final Docked Energy                 =  -10.34 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =   -9.84 kcal/mol
USER    (2) Final Internal Energy of Ligand =   -0.50 kcal/mol
USER    (3) Torsional Free Energy           =   +2.18 kcal/mol
USER
USER
USER    DPF = test.dpf
USER    NEWDPF move udp_tr.pdbq
USER    NEWDPF about16.792999 18.735001 34.970001
USER    NEWDPF tran016.863568 19.504418 34.934969
USER    NEWDPF quat0-0.617758 -0.594434 0.514804 13.202837
USER    NEWDPF ndihe7
USER    NEWDPF dihe0102.16 43.08 -71.59 8.44 90.61 -97.23 107.68
USER
USER                    Rank         x       y       z       vdW    Elec      q     RMS
ATOM      1  N1  UDP     1      18.441  20.239  33.409    -0.35  -0.11  -0.211  2.223
ATOM      2  C2  UDP     1      18.760  21.507  33.012    -0.82  +0.30  +0.396  2.223
ATOM      3  N3  UDP     1      20.096  21.792  32.894    -0.54  -0.41  -0.440  2.223
ATOM      4  H3  UDP     1      20.345  22.750  32.610    +0.03  +0.62  +0.440  2.223
ATOM      5  C4  UDP     1      21.152  20.908  33.122    -0.74  +0.29  +0.396  2.223
ATOM      6  C5  UDP     1      20.753  19.597  33.528    -0.53  +0.00  +0.000  2.223
ATOM      7  C6  UDP     1      19.448  19.308  33.641    -0.47  +0.00  +0.000  2.223
ATOM      8  O2  UDP     1      17.894  22.354  32.785    -0.28  -0.32  -0.396  2.223
ATOM      9  O4  UDP     1      22.301  21.325  32.979    -0.25  -0.27  -0.396  2.223
ATOM     10  C1' UDP     1      17.028  19.872  33.570    -0.63  +0.09  +0.324  2.223
ATOM     11  C2' UDP     1      16.614  18.599  32.829    -0.59  +0.00  +0.113  2.223
ATOM     12  C3' UDP     1      15.364  18.194  33.644    -0.63  +0.00  +0.113  2.223
ATOM     13  C4' UDP     1      15.692  18.654  35.064    -0.55  +0.03  +0.113  2.223
ATOM     14  O4' UDP     1      16.864  19.504  34.935    -0.04  -0.08  -0.227  2.223
ATOM     15  O2' UDP     1      16.246  18.896  31.502    -0.24  +0.12  -0.537  2.223
ATOM     16  HO2'UDP     1      16.994  18.596  30.862    -0.02  -0.03  +0.424  2.223
ATOM     17  O3' UDP     1      14.267  18.955  33.133    -0.24  +0.16  -0.537  2.223
ATOM     18  HO3'UDP     1      14.607  19.611  32.416    -0.21  -0.28  +0.424  2.223
ATOM     19  C5' UDP     1      16.032  17.497  36.004    -0.41  +0.04  +0.113  2.223
ATOM     20  O5' UDP     1      16.661  18.039  37.150    -0.03  -0.15  -0.368  2.223
ATOM     21  PA  UDP     1      16.337  17.982  38.693    -0.68  +0.40  +1.019  2.223
ATOM     22  O1A UDP     1      17.627  18.086  39.432    -0.25  -0.04  -0.255  2.223
ATOM     23  O2A UDP     1      15.266  18.983  38.992    -0.19  -0.11  -0.255  2.223
ATOM     24  O3A UDP     1      15.837  16.467  38.690    +0.00  -0.22  -0.510  2.223
ATOM     25  PB  UDP     1      15.882  15.298  39.781    -0.65  +0.39  +1.019  2.223
ATOM     26  O1B UDP     1      14.585  14.389  39.460    -0.02  -0.10  -0.255  2.223
ATOM     27  O2B UDP     1      15.706  16.076  41.033    -0.62  -0.20  -0.255  2.223
ATOM     28  O3B UDP     1      17.026  14.363  39.633    +0.04  -0.05  -0.255  2.223
TER
ENDMDL
```

Table 6

Residue number will be set to the conformation's cluster rank.

```
MODEL        32
USER    Run = 32
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 3
USER
USER    RMSD from reference structure       = 2.229 A
USER
USER    Estimated Free Energy of Binding    =   -9.58 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +9.46e-08       [Temperature = 298.15
K]
USER
USER    Final Docked Energy                 =  -13.09 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -13.94 kcal/mol
USER    (2) Final Internal Energy of Ligand =   +0.85 kcal/mol
USER    (3) Torsional Free Energy           =   +4.36 kcal/mol
USER
USER
USER    DPF = udp_gal.dpf
USER    NEWDPF move udp_gal.pdbq
USER    NEWDPF about15.798000 16.955999 35.483002
USER    NEWDPF tran015.935308 17.497402 35.985764
USER    NEWDPF quat0-0.511638 0.842288 -0.169640 -0.016065
USER    NEWDPF ndihe14
USER    NEWDPF dihe00.72 72.20 174.47 61.19 -168.15 179.54 -19.00 -11.55 -110.12 -5.97
49.04 165.23 96.49 -141.60
USER
USER                    Rank      x       y       z     vdW    Elec       q     RMS
ATOM      1  N   UD1     1      18.011  20.255  33.276  -0.38  -0.10  -0.211  2.229
ATOM      2  C   UD1     1      18.286  21.586  32.961  -0.84  +0.28  +0.396  2.229
ATOM      3  N1  UD1     1      19.609  21.849  32.689  -0.54  -0.39  -0.440  2.229
ATOM      4  C1  UD1     1      20.671  20.940  32.698  -0.73  +0.25  +0.396  2.229
ATOM      5  C2  UD1     1      20.312  19.592  33.032  -0.54  +0.00  +0.000  2.229
ATOM      6  C3  UD1     1      19.024  19.298  33.304  -0.47  +0.00  +0.000  2.229
ATOM      7  O   UD1     1      17.428  22.465  32.926  -0.30  -0.31  -0.396  2.229
ATOM      8  O1  UD1     1      21.808  21.330  32.427  -0.18  -0.17  -0.396  2.229
ATOM      9  C4  UD1     1      16.615  19.895  33.578  -0.65  +0.06  +0.324  2.229
ATOM     10  C5  UD1     1      16.077  18.680  32.819  -0.65  -0.01  +0.113  2.229
ATOM     11  C6  UD1     1      14.956  18.216  33.749  -0.68  +0.00  +0.113  2.229
ATOM     12  C7  UD1     1      15.422  18.644  35.144  -0.56  +0.03  +0.113  2.229
ATOM     13  O2  UD1     1      16.524  19.565  34.947  -0.06  -0.07  -0.227  2.229
ATOM     14  H1  UD1     1      19.844  22.824  32.454  +0.05  +0.64  +0.440  2.229
ATOM     15  O3  UD1     1      15.662  19.025  31.511  -0.23  +0.22  -0.537  2.229
ATOM     16  HO3 UD1     1      15.060  18.283  31.134  -0.10  -0.57  +0.424  2.229
ATOM     17  O4  UD1     1      13.664  18.758  33.445  -0.27  +0.02  -0.537  2.229
ATOM     18  HO4 UD1     1      13.725  19.337  32.597  -0.33  -0.27  +0.424  2.229
ATOM     19  C8  UD1     1      15.935  17.497  35.986  -0.36  +0.04  +0.113  2.229
ATOM     20  O5  UD1     1      16.536  18.003  37.186  -0.03  -0.15  -0.368  2.229
ATOM     21  PA  UD1     1      17.675  17.188  37.959  -0.61  +0.28  +1.019  2.229
ATOM     22  O1A UD1     1      18.860  18.071  37.912  -0.04  +0.00  -0.255  2.229
ATOM     23  O2A UD1     1      17.936  15.914  37.242  +0.05  -0.11  -0.255  2.229
ATOM     24  O3A UD1     1      17.175  16.955  39.357  -0.22  -0.14  -0.510  2.229
ATOM     25  PB  UD1     1      15.787  16.521  39.969  -0.81  +0.51  +1.019  2.229
ATOM     26  O1B UD1     1      14.830  17.653  40.007  -0.25  -0.14  -0.255  2.229
ATOM     27  O2B UD1     1      15.957  15.846  41.284  -0.64  -0.22  -0.255  2.229
ATOM     28  O6  UD1     1      15.245  15.340  39.034  +0.01  -0.16  -0.368  2.229
ATOM     29  C9  UD1     1      15.995  14.191  38.694  -0.41  +0.12  +0.227  2.229
ATOM     30  C14 UD1     1      15.190  13.345  37.718  -0.35  +0.09  +0.113  2.229
ATOM     31  O11 UD1     1      15.060  14.028  36.445  -0.27  -0.77  -0.537  2.229
ATOM     32  H11 UD1     1      15.628  14.888  36.456  +0.08  +0.38  +0.424  2.229
ATOM     33  C13 UD1     1      13.829  13.117  38.359  -0.45  +0.06  +0.113  2.229
ATOM     34  O10 UD1     1      13.011  12.358  37.481  -0.06  -0.19  -0.537  2.229
ATOM     35  HO10UD1     1      13.199  12.641  36.508  -0.03  +0.02  +0.424  2.229
```

```
ATOM     36  C12 UD1     1      13.978  12.379  39.705    -0.48  +0.09  +0.113  2.229
ATOM     37  O122UD1     1      14.315  11.027  39.382    +0.05  -0.41  -0.537  2.229
ATOM     38  H122UD1     1      13.665  10.671  38.667    +0.09  +0.30  +0.424  2.229
ATOM     39  C10 UD1     1      15.087  12.960  40.605    -0.58  +0.07  +0.113  2.229
ATOM     40  C11 UD1     1      15.535  11.852  41.547    -0.54  +0.09  +0.113  2.229
ATOM     41  O8  UD1     1      16.047  10.737  40.847    +0.01  -0.38  -0.537  2.229
ATOM     42  H8  UD1     1      15.411   9.934  40.964    +0.09  +0.33  +0.424  2.229
ATOM     43  O7  UD1     1      16.258  13.366  39.840    +0.01  -0.09  -0.227  2.229
TER
ENDMDL
MODEL       22
USER    Run = 22
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 3
USER
USER    RMSD from reference structure       = 2.268 A
USER
USER    Estimated Free Energy of Binding    =   -9.61 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +9.10e-08       [Temperature = 298.15
K]
USER
USER    Final Docked Energy                 =  -12.75 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -13.96 kcal/mol
USER    (2) Final Internal Energy of Ligand =   +1.21 kcal/mol
USER    (3) Torsional Free Energy           =   +4.36 kcal/mol
USER
USER
USER    DPF = udp_gal.dpf
USER    NEWDPF move udp_gal.pdbq
USER    NEWDPF about15.798000 16.955999 35.483002
USER    NEWDPF tran015.906499 17.202339 35.526945
USER    NEWDPF quat0-0.557219 0.582353 -0.591922 -6.199978
USER    NEWDPF ndihel4
USER    NEWDPF dihe0-60.31 98.78 176.75 -59.94 -135.34 13.12 -121.85 63.91 -96.51 -
178.60 -155.47 -91.96 33.25 179.90
USER
USER                Rank       x       y       z      vdW     Elec       q     RMS
ATOM      1  N   UD1     1      17.957  20.246  33.121    -0.38  -0.09  -0.211  2.268
ATOM      2  C   UD1     1      18.162  21.609  32.903    -0.86  +0.27  +0.396  2.268
ATOM      3  N1  UD1     1      19.479  21.969  32.733    -0.53  -0.42  -0.440  2.268
ATOM      4  C1  UD1     1      20.596  21.129  32.758    -0.75  +0.27  +0.396  2.268
ATOM      5  C2  UD1     1      20.307  19.743  32.989    -0.55  +0.00  +0.000  2.268
ATOM      6  C3  UD1     1      19.027  19.354  33.159    -0.49  +0.00  +0.000  2.268
ATOM      7  O   UD1     1      17.252  22.433  32.863    -0.31  -0.29  -0.396  2.268
ATOM      8  O1  UD1     1      21.720  21.605  32.583    -0.15  -0.19  -0.396  2.268
ATOM      9  C4  UD1     1      16.572  19.782  33.312    -0.66  +0.04  +0.324  2.268
ATOM     10  C5  UD1     1      16.162  18.585  32.450    -0.67  -0.02  +0.113  2.268
ATOM     11  C6  UD1     1      15.020  17.996  33.277    -0.68  -0.02  +0.113  2.268
ATOM     12  C7  UD1     1      15.371  18.365  34.722    -0.58  +0.02  +0.113  2.268
ATOM     13  O2  UD1     1      16.420  19.363  34.650    -0.05  -0.06  -0.227  2.268
ATOM     14  H1  UD1     1      19.664  22.970  32.570    +0.04  +0.77  +0.440  2.268
ATOM     15  O3  UD1     1      15.806  18.985  31.140    -0.12  +0.22  -0.537  2.268
ATOM     16  HO3 UD1     1      16.228  18.342  30.458    -0.28  -0.17  +0.424  2.268
ATOM     17  O4  UD1     1      13.716  18.475  32.923    -0.40  +0.06  -0.537  2.268
ATOM     18  HO4 UD1     1      13.699  18.716  31.922    -0.19  -0.26  +0.424  2.268
ATOM     19  C8  UD1     1      15.906  17.202  35.527    -0.37  +0.04  +0.113  2.268
ATOM     20  O5  UD1     1      17.089  17.601  36.234    +0.04  -0.15  -0.368  2.268
ATOM     21  PA  UD1     1      17.403  17.064  37.708    -0.55  +0.34  +1.019  2.268
ATOM     22  O1A UD1     1      17.928  18.244  38.428    -0.21  -0.04  -0.255  2.268
ATOM     23  O2A UD1     1      18.429  15.994  37.630    -0.01  -0.09  -0.255  2.268
ATOM     24  O3A UD1     1      16.106  16.562  38.278    +0.01  -0.21  -0.510  2.268
ATOM     25  PB  UD1     1      15.593  16.256  39.738    -0.72  +0.45  +1.019  2.268
ATOM     26  O1B UD1     1      14.588  17.251  40.183    -0.20  -0.12  -0.255  2.268
ATOM     27  O2B UD1     1      16.724  16.091  40.690    -0.56  -0.16  -0.255  2.268
ATOM     28  O6  UD1     1      14.962  14.786  39.682    -0.05  -0.13  -0.368  2.268
ATOM     29  C9  UD1     1      15.709  13.612  39.431    -0.46  +0.11  +0.227  2.268
ATOM     30  C14 UD1     1      15.519  13.206  37.976    -0.34  +0.09  +0.113  2.268
```

```
ATOM     31  O11 UD1     1      16.144  14.175  37.095    -0.10  -0.54  -0.537  2.268
ATOM     32  H11 UD1     1      16.693  14.844  37.654    +0.10  +0.25  +0.424  2.268
ATOM     33  C13 UD1     1      14.018  13.134  37.737    -0.43  +0.06  +0.113  2.268
ATOM     34  O10 UD1     1      13.769  12.792  36.381    -0.30  -0.27  -0.537  2.268
ATOM     35  HO10UD1     1      12.822  13.098  36.118    -0.17  -0.23  +0.424  2.268
ATOM     36  C12 UD1     1      13.367  12.093  38.668    -0.48  +0.07  +0.113  2.268
ATOM     37  O122UD1     1      13.748  10.812  38.160    +0.00  -0.35  -0.537  2.268
ATOM     38  H122UD1     1      14.102  10.914  37.199    +0.07  +0.27  +0.424  2.268
ATOM     39  C10 UD1     1      13.837  12.199  40.133    -0.49  +0.11  +0.113  2.268
ATOM     40  C11 UD1     1      13.635  10.835  40.776    -0.33  +0.15  +0.113  2.268
ATOM     41  O8  UD1     1      12.399  10.256  40.411    -0.13  -0.83  -0.537  2.268
ATOM     42  H8  UD1     1      12.486   9.812  39.484    +0.09  +0.39  +0.424  2.268
ATOM     43  O7  UD1     1      15.257  12.509  40.232    +0.00  -0.15  -0.227  2.268
TER
ENDMDL
MODEL       38
USER    Run = 38
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 3
USER
USER    RMSD from reference structure       = 2.343 A
USER
USER    Estimated Free Energy of Binding    =   -8.52 kcal/mol  [=(1)+(3)]
USER    Estimated Inhibition Constant, Ki   =   +5.73e-07       [Temperature = 298.15
K]
USER
USER    Final Docked Energy                 =  -11.93 kcal/mol  [=(1)+(2)]
USER
USER    (1) Final Intermolecular Energy     =  -12.87 kcal/mol
USER    (2) Final Internal Energy of Ligand =   +0.95 kcal/mol
USER    (3) Torsional Free Energy           =   +4.36 kcal/mol
USER
USER
USER    DPF = udp_gal.dpf
USER    NEWDPF move udp_gal.pdbq
USER    NEWDPF about15.798000 16.955999 35.483002
USER    NEWDPF tran016.468929 17.225999 35.649499
USER    NEWDPF quat00.571135 -0.378482 -0.728393 4.119217
USER    NEWDPF ndihe14
USER    NEWDPF dihe0135.84 72.34 72.68 26.52 178.87 20.84 -19.04 11.86 -120.48 46.73 -
26.80 160.70 125.77 -111.68
USER
USER                    Rank        x       y       z       vdW    Elec     q     RMS
ATOM      1  N   UD1     1      18.760  19.976  33.111    -0.33  -0.11  -0.211  2.343
ATOM      2  C   UD1     1      19.112  21.303  32.859    -0.78  +0.28  +0.396  2.343
ATOM      3  N1  UD1     1      20.454  21.506  32.633    -0.52  -0.31  -0.440  2.343
ATOM      4  C1  UD1     1      21.467  20.543  32.632    -0.71  +0.23  +0.396  2.343
ATOM      5  C2  UD1     1      21.029  19.203  32.900    -0.51  +0.00  +0.000  2.343
ATOM      6  C3  UD1     1      19.721  18.967  33.126    -0.45  +0.00  +0.000  2.343
ATOM      7  O   UD1     1      18.302  22.227  32.838    -0.27  -0.35  -0.396  2.343
ATOM      8  O1  UD1     1      22.630  20.883  32.406    -0.25  -0.23  -0.396  2.343
ATOM      9  C4  UD1     1      17.339  19.679  33.362    -0.60  +0.10  +0.324  2.343
ATOM     10  C5  UD1     1      16.760  18.526  32.539    -0.60  +0.00  +0.113  2.343
ATOM     11  C6  UD1     1      15.591  18.084  33.420    -0.60  -0.01  +0.113  2.343
ATOM     12  C7  UD1     1      16.040  18.432  34.843    -0.51  +0.03  +0.113  2.343
ATOM     13  O2  UD1     1      17.193  19.299  34.713    -0.01  -0.09  -0.227  2.343
ATOM     14  H1  UD1     1      20.746  22.476  32.445    +0.05  +0.37  +0.440  2.343
ATOM     15  O3  UD1     1      16.401  18.945  31.237    -0.21  +0.10  -0.537  2.343
ATOM     16  HO3 UD1     1      16.159  19.943  31.251    +0.00  -0.04  +0.424  2.343
ATOM     17  O4  UD1     1      14.338  18.706  33.106    -0.27  +0.13  -0.537  2.343
ATOM     18  HO4 UD1     1      14.452  19.313  32.282    -0.18  -0.28  +0.424  2.343
ATOM     19  C8  UD1     1      16.469  17.226  35.649    -0.37  +0.04  +0.113  2.343
ATOM     20  O5  UD1     1      16.397  17.525  37.051    +0.02  -0.15  -0.368  2.343
ATOM     21  PA  UD1     1      17.665  17.350  38.010    -0.63  +0.27  +1.019  2.343
ATOM     22  O1A UD1     1      18.004  18.726  38.431    +0.15  -0.04  -0.255  2.343
ATOM     23  O2A UD1     1      18.780  16.744  37.239    +0.13  -0.09  -0.255  2.343
ATOM     24  O3A UD1     1      17.232  16.478  39.155    -0.15  -0.13  -0.510  2.343
ATOM     25  PB  UD1     1      15.873  16.279  39.930    -0.78  +0.49  +1.019  2.343
```

```
ATOM     26  O1B UD1     1      15.020  17.490  39.856  -0.23  -0.13  -0.255  2.343
ATOM     27  O2B UD1     1      16.103  15.802  41.320  -0.58  -0.22  -0.255  2.343
ATOM     28  O6  UD1     1      15.153  15.026  39.242  -0.03  -0.15  -0.368  2.343
ATOM     29  C9  UD1     1      15.824  13.846  38.846  -0.41  +0.12  +0.227  2.343
ATOM     30  C14 UD1     1      15.066  13.208  37.691  -0.36  +0.09  +0.113  2.343
ATOM     31  O11 UD1     1      15.159  14.040  36.505  -0.26  -0.76  -0.537  2.343
ATOM     32  H11 UD1     1      14.326  14.642  36.442  +0.03  +0.20  +0.424  2.343
ATOM     33  C13 UD1     1      13.621  13.062  38.146  -0.46  +0.06  +0.113  2.343
ATOM     34  O10 UD1     1      12.847  12.501  37.096  -0.10  -0.09  -0.537  2.343
ATOM     35  HO10UD1     1      12.729  13.199  36.347  -0.12  -0.17  +0.424  2.343
ATOM     36  C12 UD1     1      13.533  12.167  39.398  -0.49  +0.09  +0.113  2.343
ATOM     37  O122UD1     1      13.775  10.831  38.949  +0.03  -0.40  -0.537  2.343
ATOM     38  H122UD1     1      13.044  10.555  38.279  +0.09  +0.28  +0.424  2.343
ATOM     39  C10 UD1     1      14.576  12.517  40.479  -0.51  +0.09  +0.113  2.343
ATOM     40  C11 UD1     1      14.796  11.268  41.320  -0.33  +0.12  +0.113  2.343
ATOM     41  O8  UD1     1      15.279  10.188  40.548  +0.04  -0.41  -0.537  2.343
ATOM     42  H8  UD1     1      16.309  10.214  40.524  +0.09  +0.29  +0.424  2.343
ATOM     43  O7  UD1     1      15.865  12.874  39.903  +0.01  -0.12  -0.227  2.343
TER
ENDMDL
```

Table 7

Uracil											
ATOM	1	N1	UDP	1	18.167	20.363	33.367	-0.38	-0.11	-0.211	2.450
ATOM	2	C2	UDP	1	18.485	21.574	32.818	-0.84	+0.28	+0.396	2.450
ATOM	3	N3	UDP	1	19.821	21.872	32.732	-0.53	-0.40	-0.440	2.450
ATOM	4	H3	UDP	1	20.069	22.789	32.334	+0.07	+0.53	+0.440	2.450
ATOM	5	C4	UDP	1	20.878	21.052	33.133	-0.75	+0.30	+0.396	2.450
ATOM	6	C5	UDP	1	20.479	19.798	33.691	-0.55	+0.00	+0.000	2.450
ATOM	7	C6	UDP	1	19.174	19.496	33.774	-0.49	+0.00	+0.000	2.450
ATOM	8	O2	UDP	1	17.619	22.362	32.433	-0.35	-0.26	-0.396	2.450
ATOM	9	O4	UDP	1	22.026	21.474	32.994	-0.24	-0.27	-0.396	2.450
Ribose											
ATOM	10	C1'	UDP	1	16.753	19.988	33.503	-0.65	+0.07	+0.324	2.450
ATOM	11	C2'	UDP	1	16.402	18.617	32.920	-0.60	+0.00	+0.113	2.450
ATOM	12	C3'	UDP	1	15.116	18.296	33.717	-0.67	+0.00	+0.113	2.450
ATOM	13	C4'	UDP	1	15.358	18.950	35.076	-0.56	+0.02	+0.113	2.450
ATOM	14	O4'	UDP	1	16.521	19.804	34.894	-0.07	-0.07	-0.227	2.450
ATOM	15	O2'	UDP	1	16.102	18.725	31.548	-0.24	+0.17	-0.537	2.450
ATOM	16	HO2'	UDP	1	15.697	17.839	31.214	-0.28	-0.47	+0.424	2.450
ATOM	17	O3'	UDP	1	14.035	18.955	33.051	-0.27	+0.16	-0.537	2.450
ATOM	18	HO3'	UDP	1	14.102	18.785	32.037	-0.17	-0.28	+0.424	2.450
ATOM	19	C5'	UDP	1	15.666	17.939	36.181	-0.30	+0.04	+0.113	2.450
ATOM	20	O5'	UDP	1	15.126	18.439	37.390	+0.00	-0.18	-0.368	2.450
Pyrophosphate											
ATOM	21	PA	UDP	1	15.642	18.457	38.881	-0.61	+0.45	+1.019	2.450
ATOM	22	O1A	UDP	1	17.132	18.480	38.845	-0.15	-0.08	-0.255	2.450
ATOM	23	O2A	UDP	1	14.933	19.550	39.617	-0.24	-0.09	-0.255	2.450
ATOM	24	O3A	UDP	1	15.133	16.987	39.239	-0.07	-0.23	-0.510	2.450
ATOM	25	PB	UDP	1	15.835	15.723	39.920	-0.72	+0.43	+1.019	2.450
ATOM	26	O1B	UDP	1	15.020	14.448	39.353	-0.03	-0.11	-0.255	2.450
ATOM	27	O2B	UDP	1	15.532	15.971	41.352	-0.68	-0.23	-0.255	2.450
ATOM	28	O3B	UDP	1	17.233	15.484	39.480	-0.12	-0.06	-0.255	2.450

Table 8

REMARK 4 1GAL COMPLIES WITH FORMAT V. 2.0, 12-JAN-2000

ATOM	1	N	GLN	125	3.774	29.638	36.504	1.00	0.00		N
ATOM	2	CA	GLN	125	2.861	28.997	35.607	1.00	0.00		C
ATOM	3	C	GLN	125	3.659	28.369	34.516	1.00	0.00		C
ATOM	4	O	GLN	125	3.480	27.195	34.201	1.00	0.00		O
ATOM	5	CB	GLN	125	1.885	29.988	34.950	1.00	0.00		C
ATOM	6	CG	GLN	125	0.963	30.690	35.948	1.00	0.00		C
ATOM	7	CD	GLN	125	0.056	31.635	35.172	1.00	0.00		C
ATOM	8	OE1	GLN	125	-0.698	32.411	35.755	1.00	0.00		O
ATOM	9	NE2	GLN	125	0.131	31.571	33.815	1.00	0.00		N
ATOM	10	1H	GLN	125	4.428	30.225	35.967	1.00	0.00		H
ATOM	11	2H	GLN	125	3.249	30.226	37.166	1.00	0.00		H
ATOM	12	HA	GLN	125	2.310	28.245	36.172	1.00	0.00		H
ATOM	13	1HB	GLN	125	1.217	29.524	34.223	1.00	0.00		H
ATOM	14	2HB	GLN	125	2.381	30.792	34.407	1.00	0.00		H
ATOM	15	1HG	GLN	125	1.583	31.242	36.653	1.00	0.00		H
ATOM	16	2HG	GLN	125	0.377	29.928	36.463	1.00	0.00		H
ATOM	17	1HE2	GLN	125	-0.457	32.187	33.237	1.00	0.00		H
ATOM	18	2HE2	GLN	125	0.776	30.906	33.365	1.00	0.00		H
ATOM	19	N	LYS	126	4.583	29.141	33.917	1.00	0.00		N
ATOM	20	CA	LYS	126	5.373	28.597	32.859	1.00	0.00		C
ATOM	21	C	LYS	126	6.430	27.759	33.485	1.00	0.00		C
ATOM	22	O	LYS	126	6.743	27.906	34.665	1.00	0.00		O
ATOM	23	CB	LYS	126	6.036	29.676	31.992	1.00	0.00		C
ATOM	24	CG	LYS	126	5.011	30.426	31.142	1.00	0.00		C
ATOM	25	CD	LYS	126	3.953	31.165	31.965	1.00	0.00		C
ATOM	26	CE	LYS	126	4.502	32.348	32.763	1.00	0.00		C
ATOM	27	NZ	LYS	126	3.406	33.004	33.511	1.00	0.00		N
ATOM	28	H	LYS	126	4.719	30.116	34.218	1.00	0.00		H
ATOM	29	HA	LYS	126	4.707	28.002	32.232	1.00	0.00		H
ATOM	30	1HB	LYS	126	6.769	29.248	31.308	1.00	0.00		H
ATOM	31	2HB	LYS	126	6.555	30.417	32.599	1.00	0.00		H
ATOM	32	1HG	LYS	126	4.444	29.781	30.469	1.00	0.00		H
ATOM	33	2HG	LYS	126	5.450	31.188	30.498	1.00	0.00		H
ATOM	34	1HD	LYS	126	3.514	30.461	32.672	1.00	0.00		H
ATOM	35	2HD	LYS	126	3.192	31.546	31.283	1.00	0.00		H
ATOM	36	1HE	LYS	126	4.954	33.073	32.087	1.00	0.00		H
ATOM	37	2HE	LYS	126	5.256	32.001	33.469	1.00	0.00		H
ATOM	38	1HZ	LYS	126	2.520	32.513	33.323	1.00	0.00		H
ATOM	39	2HZ	LYS	126	3.609	32.970	34.520	1.00	0.00		H
ATOM	40	3HZ	LYS	126	3.324	33.985	33.210	1.00	0.00		H
ATOM	41	N	ILE	127	6.994	26.817	32.713	1.00	0.00		N
ATOM	42	CA	ILE	127	7.996	25.997	33.310	1.00	0.00		C
ATOM	43	C	ILE	127	9.165	25.944	32.400	1.00	0.00		C
ATOM	44	O	ILE	127	9.040	26.043	31.181	1.00	0.00		O
ATOM	45	CB	ILE	127	7.575	24.578	33.539	1.00	0.00		C
ATOM	46	CG1	ILE	127	8.654	23.841	34.351	1.00	0.00		C
ATOM	47	CG2	ILE	127	7.271	23.937	32.176	1.00	0.00		C
ATOM	48	CD1	ILE	127	8.211	22.470	34.856	1.00	0.00		C
ATOM	49	H	ILE	127	6.714	26.691	31.729	1.00	0.00		H
ATOM	50	HA	ILE	127	8.278	26.436	34.266	1.00	0.00		H
ATOM	51	HB	ILE	127	6.684	24.581	34.167	1.00	0.00		H
ATOM	52	1HG1	ILE	127	8.974	24.379	35.242	1.00	0.00		H
ATOM	53	2HG1	ILE	127	9.570	23.652	33.791	1.00	0.00		H
ATOM	54	1HG2	ILE	127	7.435	24.668	31.385	1.00	0.00		H
ATOM	55	2HG2	ILE	127	7.928	23.081	32.021	1.00	0.00		H
ATOM	56	3HG2	ILE	127	6.232	23.605	32.153	1.00	0.00		H
ATOM	57	1HD1	ILE	127	7.188	22.276	34.533	1.00	0.00		H
ATOM	58	2HD1	ILE	127	8.870	21.702	34.451	1.00	0.00		H
ATOM	59	3HD1	ILE	127	8.257	22.450	35.944	1.00	0.00		H
ATOM	60	N	THR	128	10.355	25.811	33.002	1.00	0.00		N
ATOM	61	CA	THR	128	11.546	25.664	32.234	1.00	0.00		C
ATOM	62	C	THR	128	11.987	24.261	32.465	1.00	0.00		C
ATOM	63	O	THR	128	12.094	23.810	33.605	1.00	0.00		O

ATOM	64	CB	THR	128	12.634	26.603	32.656	1.00	0.00	C
ATOM	65	OG1	THR	128	12.906	26.435	34.037	1.00	0.00	O
ATOM	66	CG2	THR	128	12.179	28.044	32.377	1.00	0.00	C
ATOM	67	H	THR	128	10.409	25.815	34.030	1.00	0.00	H
ATOM	68	HA	THR	128	11.246	25.860	31.204	1.00	0.00	H
ATOM	69	HB	THR	128	13.534	26.375	32.084	1.00	0.00	H
ATOM	70	HG1	THR	128	12.856	27.348	34.510	1.00	0.00	H
ATOM	71	1HG2	THR	128	11.179	28.032	31.941	1.00	0.00	H
ATOM	72	2HG2	THR	128	12.161	28.607	33.310	1.00	0.00	H
ATOM	73	3HG2	THR	128	12.872	28.516	31.680	1.00	0.00	H
ATOM	74	N	VAL	129	12.221	23.517	31.369	1.00	0.00	N
ATOM	75	CA	VAL	129	12.615	22.148	31.497	1.00	0.00	C
ATOM	76	C	VAL	129	14.091	22.103	31.268	1.00	0.00	C
ATOM	77	O	VAL	129	14.601	22.747	30.358	1.00	0.00	O
ATOM	78	CB	VAL	129	11.961	21.255	30.478	1.00	0.00	C
ATOM	79	CG1	VAL	129	12.454	19.813	30.683	1.00	0.00	C
ATOM	80	CG2	VAL	129	10.434	21.408	30.611	1.00	0.00	C
ATOM	81	H	VAL	129	12.116	23.935	30.433	1.00	0.00	H
ATOM	82	HA	VAL	129	12.347	21.838	32.507	1.00	0.00	H
ATOM	83	HB	VAL	129	12.228	21.599	29.478	1.00	0.00	H
ATOM	84	1HG1	VAL	129	13.157	19.783	31.515	1.00	0.00	H
ATOM	85	2HG1	VAL	129	11.604	19.165	30.902	1.00	0.00	H
ATOM	86	3HG1	VAL	129	12.949	19.465	29.776	1.00	0.00	H
ATOM	87	1HG2	VAL	129	10.207	22.120	31.404	1.00	0.00	H
ATOM	88	2HG2	VAL	129	10.021	21.770	29.669	1.00	0.00	H
ATOM	89	3HG2	VAL	129	9.991	20.441	30.853	1.00	0.00	H
ATOM	90	N	GLY	130	14.827	21.351	32.109	1.00	0.00	N
ATOM	91	CA	GLY	130	16.251	21.295	31.941	1.00	0.00	C
ATOM	92	C	GLY	130	16.576	19.918	31.483	1.00	0.00	C
ATOM	93	O	GLY	130	16.223	18.933	32.129	1.00	0.00	O
ATOM	94	H	GLY	130	14.371	20.821	32.865	1.00	0.00	H
ATOM	95	1HA	GLY	130	16.691	21.516	32.912	1.00	0.00	H
ATOM	96	2HA	GLY	130	16.509	22.045	31.194	1.00	0.00	H
ATOM	97	N	LEU	131	17.293	19.816	30.350	1.00	0.00	N
ATOM	98	CA	LEU	131	17.552	18.511	29.838	1.00	0.00	C
ATOM	99	C	LEU	131	19.040	18.385	29.719	1.00	0.00	C
ATOM	100	O	LEU	131	19.709	19.308	29.260	1.00	0.00	O
ATOM	101	CB	LEU	131	16.969	18.330	28.430	1.00	0.00	C
ATOM	102	CG	LEU	131	16.783	16.855	28.071	1.00	0.00	C
ATOM	103	CD1	LEU	131	15.603	16.268	28.862	1.00	0.00	C
ATOM	104	CD2	LEU	131	16.663	16.648	26.550	1.00	0.00	C
ATOM	105	H	LEU	131	17.644	20.655	29.866	1.00	0.00	H
ATOM	106	HA	LEU	131	17.135	17.805	30.557	1.00	0.00	H
ATOM	107	1HB	LEU	131	17.611	18.762	27.662	1.00	0.00	H
ATOM	108	2HB	LEU	131	15.993	18.804	28.327	1.00	0.00	H
ATOM	109	HG	LEU	131	17.686	16.296	28.314	1.00	0.00	H
ATOM	110	1HD1	LEU	131	15.170	17.040	29.497	1.00	0.00	H
ATOM	111	2HD1	LEU	131	14.845	15.903	28.168	1.00	0.00	H
ATOM	112	3HD1	LEU	131	15.954	15.443	29.481	1.00	0.00	H
ATOM	113	1HD2	LEU	131	16.737	17.611	26.044	1.00	0.00	H
ATOM	114	2HD2	LEU	131	17.466	15.995	26.207	1.00	0.00	H
ATOM	115	3HD2	LEU	131	15.700	16.190	26.319	1.00	0.00	H
ATOM	116	N	THR	132	19.607	17.244	30.157	1.00	0.00	N
ATOM	117	CA	THR	132	21.018	17.037	30.005	1.00	0.00	C
ATOM	118	C	THR	132	21.177	15.992	28.951	1.00	0.00	C
ATOM	119	O	THR	132	20.496	14.967	28.976	1.00	0.00	O
ATOM	120	CB	THR	132	21.706	16.558	31.252	1.00	0.00	C
ATOM	121	OG1	THR	132	21.133	15.339	31.699	1.00	0.00	O
ATOM	122	CG2	THR	132	21.583	17.642	32.338	1.00	0.00	C
ATOM	123	H	THR	132	19.026	16.519	30.601	1.00	0.00	H
ATOM	124	HA	THR	132	21.437	17.997	29.705	1.00	0.00	H
ATOM	125	HB	THR	132	22.756	16.372	31.027	1.00	0.00	H
ATOM	126	HG1	THR	132	20.160	15.504	31.994	1.00	0.00	H
ATOM	127	1HG2	THR	132	21.028	18.492	31.941	1.00	0.00	H
ATOM	128	2HG2	THR	132	21.055	17.234	33.200	1.00	0.00	H
ATOM	129	3HG2	THR	132	22.578	17.967	32.641	1.00	0.00	H
ATOM	130	N	VAL	133	22.079	16.244	27.979	1.00	0.00	N
ATOM	131	CA	VAL	133	22.229	15.303	26.910	1.00	0.00	C

ATOM	132	C	VAL	133	23.665	14.894	26.786	1.00	0.00	C
ATOM	133	O	VAL	133	24.595	15.690	26.922	1.00	0.00	O
ATOM	134	CB	VAL	133	21.830	15.851	25.570	1.00	0.00	C
ATOM	135	CG1	VAL	133	20.354	16.275	25.623	1.00	0.00	C
ATOM	136	CG2	VAL	133	22.783	16.997	25.201	1.00	0.00	C
ATOM	137	H	VAL	133	22.650	17.100	28.005	1.00	0.00	H
ATOM	138	HA	VAL	133	21.624	14.417	27.105	1.00	0.00	H
ATOM	139	HB	VAL	133	21.968	15.076	24.815	1.00	0.00	H
ATOM	140	1HG1	VAL	133	19.953	16.076	26.617	1.00	0.00	H
ATOM	141	2HG1	VAL	133	20.273	17.340	25.405	1.00	0.00	H
ATOM	142	3HG1	VAL	133	19.786	15.709	24.883	1.00	0.00	H
ATOM	143	1HG2	VAL	133	23.514	17.133	25.998	1.00	0.00	H
ATOM	144	2HG2	VAL	133	23.299	16.755	24.272	1.00	0.00	H
ATOM	145	3HG2	VAL	133	22.212	17.916	25.070	1.00	0.00	H
ATOM	146	N	PHE	134	23.857	13.592	26.526	1.00	0.00	N
ATOM	147	CA	PHE	134	25.138	13.016	26.297	1.00	0.00	C
ATOM	148	C	PHE	134	24.939	12.254	25.042	1.00	0.00	C
ATOM	149	O	PHE	134	23.939	12.454	24.357	1.00	0.00	O
ATOM	150	CB	PHE	134	25.581	12.031	27.387	1.00	0.00	C
ATOM	151	CG	PHE	134	25.779	12.856	28.606	1.00	0.00	C
ATOM	152	CD1	PHE	134	24.964	12.698	29.703	1.00	0.00	C
ATOM	153	CD2	PHE	134	26.810	13.759	28.664	1.00	0.00	C
ATOM	154	CE1	PHE	134	25.156	13.454	30.834	1.00	0.00	C
ATOM	155	CE2	PHE	134	27.006	14.518	29.790	1.00	0.00	C
ATOM	156	CZ	PHE	134	26.179	14.370	30.876	1.00	0.00	C
ATOM	157	H	PHE	134	23.032	12.975	26.490	1.00	0.00	H
ATOM	158	HA	PHE	134	25.901	13.786	26.189	1.00	0.00	H
ATOM	159	1HB	PHE	134	26.504	11.585	27.015	1.00	0.00	H
ATOM	160	2HB	PHE	134	24.765	11.316	27.479	1.00	0.00	H
ATOM	161	HD1	PHE	134	24.157	11.965	29.674	1.00	0.00	H
ATOM	162	HD2	PHE	134	27.479	13.875	27.809	1.00	0.00	H
ATOM	163	HE1	PHE	134	24.500	13.328	31.695	1.00	0.00	H
ATOM	164	HE2	PHE	134	27.821	15.241	29.824	1.00	0.00	H
ATOM	165	HZ	PHE	134	26.334	14.976	31.769	1.00	0.00	H
ATOM	166	N	ALA	135	25.881	11.365	24.698	1.00	0.00	N
ATOM	167	CA	ALA	135	25.736	10.705	23.434	1.00	0.00	C
ATOM	168	C	ALA	135	24.749	9.589	23.519	1.00	0.00	C
ATOM	169	O	ALA	135	25.132	8.421	23.496	1.00	0.00	O
ATOM	170	CB	ALA	135	27.051	10.116	22.893	1.00	0.00	C
ATOM	171	H	ALA	135	26.678	11.163	25.318	1.00	0.00	H
ATOM	172	HA	ALA	135	25.389	11.396	22.666	1.00	0.00	H
ATOM	173	1HB	ALA	135	27.858	10.321	23.596	1.00	0.00	H
ATOM	174	2HB	ALA	135	26.943	9.038	22.769	1.00	0.00	H
ATOM	175	3HB	ALA	135	27.284	10.570	21.930	1.00	0.00	H
ATOM	176	N	VAL	136	23.446	9.913	23.642	1.00	0.00	N
ATOM	177	CA	VAL	136	22.465	8.870	23.562	1.00	0.00	C
ATOM	178	C	VAL	136	21.648	9.153	22.336	1.00	0.00	C
ATOM	179	O	VAL	136	20.541	9.686	22.389	1.00	0.00	O
ATOM	180	CB	VAL	136	21.574	8.768	24.772	1.00	0.00	C
ATOM	181	CG1	VAL	136	20.893	10.116	25.062	1.00	0.00	C
ATOM	182	CG2	VAL	136	20.572	7.638	24.501	1.00	0.00	C
ATOM	183	H	VAL	136	23.160	10.891	23.790	1.00	0.00	H
ATOM	184	HA	VAL	136	23.018	7.934	23.486	1.00	0.00	H
ATOM	185	HB	VAL	136	22.149	8.481	25.652	1.00	0.00	H
ATOM	186	1HG1	VAL	136	21.209	10.850	24.321	1.00	0.00	H
ATOM	187	2HG1	VAL	136	19.810	9.994	25.013	1.00	0.00	H
ATOM	188	3HG1	VAL	136	21.175	10.459	26.057	1.00	0.00	H
ATOM	189	1HG2	VAL	136	20.763	7.209	23.517	1.00	0.00	H
ATOM	190	2HG2	VAL	136	20.681	6.864	25.261	1.00	0.00	H
ATOM	191	3HG2	VAL	136	19.557	8.035	24.532	1.00	0.00	H
ATOM	192	N	GLY	137	22.180	8.741	21.176	1.00	0.00	N
ATOM	193	CA	GLY	137	21.598	9.106	19.921	1.00	0.00	C
ATOM	194	C	GLY	137	20.249	8.504	19.733	1.00	0.00	C
ATOM	195	O	GLY	137	19.339	9.157	19.228	1.00	0.00	O
ATOM	196	H	GLY	137	23.023	8.150	21.188	1.00	0.00	H
ATOM	197	1HA	GLY	137	22.206	8.781	19.077	1.00	0.00	H
ATOM	198	2HA	GLY	137	21.476	10.184	19.823	1.00	0.00	H
ATOM	199	N	ARG	138	20.103	7.223	20.105	1.00	0.00	N

ATOM	200	CA	ARG	138	18.884	6.506	19.899	1.00	0.00	C
ATOM	201	C	ARG	138	17.789	7.041	20.772	1.00	0.00	C
ATOM	202	O	ARG	138	16.648	7.142	20.331	1.00	0.00	O
ATOM	203	CB	ARG	138	19.029	5.019	20.256	1.00	0.00	C
ATOM	204	CG	ARG	138	20.086	4.283	19.440	1.00	0.00	C
ATOM	205	CD	ARG	138	19.502	3.245	18.482	1.00	0.00	C
ATOM	206	NE	ARG	138	18.334	3.855	17.782	1.00	0.00	N
ATOM	207	CZ	ARG	138	17.889	3.261	16.637	1.00	0.00	C
ATOM	208	NH1	ARG	138	18.585	2.201	16.132	1.00	0.00	N
ATOM	209	NH2	ARG	138	16.757	3.708	16.016	1.00	0.00	N
ATOM	210	H	ARG	138	20.895	6.740	20.553	1.00	0.00	H
ATOM	211	HA	ARG	138	18.552	6.584	18.863	1.00	0.00	H
ATOM	212	1HB	ARG	138	18.071	4.528	20.078	1.00	0.00	H
ATOM	213	2HB	ARG	138	19.309	4.944	21.306	1.00	0.00	H
ATOM	214	1HG	ARG	138	20.803	3.735	20.051	1.00	0.00	H
ATOM	215	2HG	ARG	138	20.688	4.941	18.814	1.00	0.00	H
ATOM	216	1HD	ARG	138	19.188	2.378	19.063	1.00	0.00	H
ATOM	217	2HD	ARG	138	20.274	2.965	17.765	1.00	0.00	H
ATOM	218	HE	ARG	138	17.876	4.700	18.152	1.00	0.00	H
ATOM	219	1HH1	ARG	138	19.430	1.863	16.614	1.00	0.00	H
ATOM	220	2HH1	ARG	138	18.265	1.739	15.268	1.00	0.00	H
ATOM	221	1HH2	ARG	138	16.231	4.500	16.411	1.00	0.00	H
ATOM	222	2HH2	ARG	138	16.429	3.252	15.152	1.00	0.00	H
ATOM	223	N	TYR	139	18.106	7.327	22.054	1.00	0.00	N
ATOM	224	CA	TYR	139	17.141	7.688	23.058	1.00	0.00	C
ATOM	225	C	TYR	139	16.701	9.138	23.118	1.00	0.00	C
ATOM	226	O	TYR	139	15.571	9.413	23.509	1.00	0.00	O
ATOM	227	CB	TYR	139	17.606	7.224	24.444	1.00	0.00	C
ATOM	228	CG	TYR	139	17.790	5.742	24.314	1.00	0.00	C
ATOM	229	CD1	TYR	139	16.725	4.947	23.963	1.00	0.00	C
ATOM	230	CD2	TYR	139	18.998	5.136	24.575	1.00	0.00	C
ATOM	231	CE1	TYR	139	16.864	3.584	23.834	1.00	0.00	C
ATOM	232	CE2	TYR	139	19.142	3.774	24.445	1.00	0.00	C
ATOM	233	CZ	TYR	139	18.081	2.988	24.068	1.00	0.00	C
ATOM	234	OH	TYR	139	18.231	1.587	23.930	1.00	0.00	O
ATOM	235	H	TYR	139	19.097	7.284	22.328	1.00	0.00	H
ATOM	236	HA	TYR	139	16.242	7.099	22.875	1.00	0.00	H
ATOM	237	1HB	TYR	139	16.798	7.505	25.120	1.00	0.00	H
ATOM	238	2HB	TYR	139	18.535	7.764	24.624	1.00	0.00	H
ATOM	239	HD1	TYR	139	15.752	5.404	23.783	1.00	0.00	H
ATOM	240	HD2	TYR	139	19.848	5.741	24.887	1.00	0.00	H
ATOM	241	HE1	TYR	139	16.007	2.975	23.545	1.00	0.00	H
ATOM	242	HE2	TYR	139	20.109	3.313	24.643	1.00	0.00	H
ATOM	243	HH	TYR	139	17.306	1.154	23.791	1.00	0.00	H
ATOM	244	N	ILE	140	17.564	10.112	22.757	1.00	0.00	N
ATOM	245	CA	ILE	140	17.287	11.521	22.936	1.00	0.00	C
ATOM	246	C	ILE	140	16.072	11.997	22.202	1.00	0.00	C
ATOM	247	O	ILE	140	15.317	12.810	22.729	1.00	0.00	O
ATOM	248	CB	ILE	140	18.430	12.394	22.498	1.00	0.00	C
ATOM	249	CG1	ILE	140	18.741	12.087	21.022	1.00	0.00	C
ATOM	250	CG2	ILE	140	19.611	12.229	23.462	1.00	0.00	C
ATOM	251	CD1	ILE	140	19.798	12.984	20.382	1.00	0.00	C
ATOM	252	H	ILE	140	18.462	9.838	22.333	1.00	0.00	H
ATOM	253	HA	ILE	140	17.130	11.708	23.998	1.00	0.00	H
ATOM	254	HB	ILE	140	18.117	13.438	22.492	1.00	0.00	H
ATOM	255	1HG1	ILE	140	17.821	12.208	20.449	1.00	0.00	H
ATOM	256	2HG1	ILE	140	19.103	11.061	20.958	1.00	0.00	H
ATOM	257	1HG2	ILE	140	19.346	11.515	24.242	1.00	0.00	H
ATOM	258	2HG2	ILE	140	20.479	11.862	22.914	1.00	0.00	H
ATOM	259	3HG2	ILE	140	19.847	13.191	23.915	1.00	0.00	H
ATOM	260	1HD1	ILE	140	20.154	13.707	21.115	1.00	0.00	H
ATOM	261	2HD1	ILE	140	20.633	12.373	20.038	1.00	0.00	H
ATOM	262	3HD1	ILE	140	19.362	13.512	19.534	1.00	0.00	H
ATOM	263	N	GLU	141	15.842	11.505	20.979	1.00	0.00	N
ATOM	264	CA	GLU	141	14.778	11.954	20.132	1.00	0.00	C
ATOM	265	C	GLU	141	13.475	11.779	20.850	1.00	0.00	C
ATOM	266	O	GLU	141	12.644	12.683	20.902	1.00	0.00	O
ATOM	267	CB	GLU	141	14.738	11.068	18.876	1.00	0.00	C

ATOM	268	CG	GLU	141	13.662	11.398	17.847	1.00	0.00	C
ATOM	269	CD	GLU	141	13.763	10.310	16.789	1.00	0.00	C
ATOM	270	OE1	GLU	141	14.828	9.634	16.753	1.00	0.00	O
ATOM	271	OE2	GLU	141	12.782	10.123	16.023	1.00	0.00	O
ATOM	272	H	GLU	141	16.464	10.763	20.627	1.00	0.00	H
ATOM	273	HA	GLU	141	14.932	13.006	19.894	1.00	0.00	H
ATOM	274	1HB	GLU	141	14.563	10.041	19.198	1.00	0.00	H
ATOM	275	2HB	GLU	141	15.699	11.163	18.371	1.00	0.00	H
ATOM	276	1HG	GLU	141	13.914	12.388	17.467	1.00	0.00	H
ATOM	277	2HG	GLU	141	12.719	11.377	18.393	1.00	0.00	H
ATOM	278	N	HIS	142	13.289	10.597	21.455	1.00	0.00	N
ATOM	279	CA	HIS	142	12.086	10.211	22.131	1.00	0.00	C
ATOM	280	C	HIS	142	11.845	11.099	23.313	1.00	0.00	C
ATOM	281	O	HIS	142	10.720	11.534	23.559	1.00	0.00	O
ATOM	282	CB	HIS	142	12.224	8.783	22.670	1.00	0.00	C
ATOM	283	CG	HIS	142	11.008	8.298	23.379	1.00	0.00	C
ATOM	284	ND1	HIS	142	10.927	7.058	23.966	1.00	0.00	N
ATOM	285	CD2	HIS	142	9.808	8.899	23.600	1.00	0.00	C
ATOM	286	CE1	HIS	142	9.691	6.968	24.514	1.00	0.00	C
ATOM	287	NE2	HIS	142	8.975	8.060	24.317	1.00	0.00	N
ATOM	288	H	HIS	142	14.064	9.919	21.432	1.00	0.00	H
ATOM	289	HA	HIS	142	11.231	10.288	21.458	1.00	0.00	H
ATOM	290	1HB	HIS	142	13.038	8.666	23.385	1.00	0.00	H
ATOM	291	2HB	HIS	142	12.416	8.043	21.892	1.00	0.00	H
ATOM	292	HD1	HIS	142	11.662	6.337	23.985	1.00	0.00	H
ATOM	293	HD2	HIS	142	9.541	9.899	23.260	1.00	0.00	H
ATOM	294	HE1	HIS	142	9.329	6.094	25.055	1.00	0.00	H
ATOM	295	HE2	HIS	142	8.010	8.245	24.628	1.00	0.00	H
ATOM	296	N	TYR	143	12.917	11.376	24.070	1.00	0.00	N
ATOM	297	CA	TYR	143	12.847	12.085	25.311	1.00	0.00	C
ATOM	298	C	TYR	143	12.362	13.475	25.001	1.00	0.00	C
ATOM	299	O	TYR	143	11.390	13.953	25.584	1.00	0.00	O
ATOM	300	CB	TYR	143	14.265	12.216	25.877	1.00	0.00	C
ATOM	301	CG	TYR	143	14.353	12.188	27.364	1.00	0.00	C
ATOM	302	CD1	TYR	143	13.642	13.019	28.204	1.00	0.00	C
ATOM	303	CD2	TYR	143	15.190	11.243	27.924	1.00	0.00	C
ATOM	304	CE1	TYR	143	13.802	12.925	29.571	1.00	0.00	C
ATOM	305	CE2	TYR	143	15.357	11.146	29.290	1.00	0.00	C
ATOM	306	CZ	TYR	143	14.662	12.001	30.119	1.00	0.00	C
ATOM	307	OH	TYR	143	14.825	11.929	31.520	1.00	0.00	O
ATOM	308	H	TYR	143	13.840	11.061	23.740	1.00	0.00	H
ATOM	309	HA	TYR	143	12.146	11.546	25.949	1.00	0.00	H
ATOM	310	1HB	TYR	143	14.676	13.168	25.543	1.00	0.00	H
ATOM	311	2HB	TYR	143	14.859	11.384	25.499	1.00	0.00	H
ATOM	312	HD1	TYR	143	12.951	13.752	27.786	1.00	0.00	H
ATOM	313	HD2	TYR	143	15.731	10.557	27.271	1.00	0.00	H
ATOM	314	HE1	TYR	143	13.240	13.591	30.225	1.00	0.00	H
ATOM	315	HE2	TYR	143	16.032	10.400	29.710	1.00	0.00	H
ATOM	316	HH	TYR	143	14.815	12.879	31.916	1.00	0.00	H
ATOM	317	N	LEU	144	13.012	14.156	24.026	1.00	0.00	N
ATOM	318	CA	LEU	144	12.699	15.521	23.676	1.00	0.00	C
ATOM	319	C	LEU	144	11.328	15.648	23.096	1.00	0.00	C
ATOM	320	O	LEU	144	10.590	16.568	23.440	1.00	0.00	O
ATOM	321	CB	LEU	144	13.708	16.137	22.693	1.00	0.00	C
ATOM	322	CG	LEU	144	15.006	16.551	23.386	1.00	0.00	C
ATOM	323	CD1	LEU	144	16.003	17.174	22.393	1.00	0.00	C
ATOM	324	CD2	LEU	144	14.667	17.512	24.538	1.00	0.00	C
ATOM	325	H	LEU	144	13.764	13.677	23.510	1.00	0.00	H
ATOM	326	HA	LEU	144	12.739	16.182	24.541	1.00	0.00	H
ATOM	327	1HB	LEU	144	13.313	17.029	22.206	1.00	0.00	H
ATOM	328	2HB	LEU	144	13.983	15.442	21.899	1.00	0.00	H
ATOM	329	HG	LEU	144	15.501	15.698	23.851	1.00	0.00	H
ATOM	330	1HD1	LEU	144	15.563	17.186	21.395	1.00	0.00	H
ATOM	331	2HD1	LEU	144	16.233	18.194	22.700	1.00	0.00	H
ATOM	332	3HD1	LEU	144	16.919	16.583	22.378	1.00	0.00	H
ATOM	333	1HD2	LEU	144	13.588	17.663	24.580	1.00	0.00	H
ATOM	334	2HD2	LEU	144	15.010	17.085	25.480	1.00	0.00	H
ATOM	335	3HD2	LEU	144	15.161	18.468	24.371	1.00	0.00	H

ATOM	336	N	GLU	145	10.934	14.706	22.226	1.00	0.00	N
ATOM	337	CA	GLU	145	9.653	14.803	21.588	1.00	0.00	C
ATOM	338	C	GLU	145	8.586	14.783	22.637	1.00	0.00	C
ATOM	339	O	GLU	145	7.560	15.453	22.512	1.00	0.00	O
ATOM	340	CB	GLU	145	9.368	13.627	20.636	1.00	0.00	C
ATOM	341	CG	GLU	145	10.226	13.647	19.371	1.00	0.00	C
ATOM	342	CD	GLU	145	9.522	14.481	18.306	1.00	0.00	C
ATOM	343	OE1	GLU	145	8.392	14.096	17.899	1.00	0.00	O
ATOM	344	OE2	GLU	145	10.111	15.506	17.874	1.00	0.00	O
ATOM	345	H	GLU	145	11.553	13.910	22.015	1.00	0.00	H
ATOM	346	HA	GLU	145	9.607	15.736	21.027	1.00	0.00	H
ATOM	347	1HB	GLU	145	8.337	13.595	20.282	1.00	0.00	H
ATOM	348	2HB	GLU	145	9.546	12.650	21.087	1.00	0.00	H
ATOM	349	1HG	GLU	145	10.358	12.625	19.015	1.00	0.00	H
ATOM	350	2HG	GLU	145	11.195	14.086	19.606	1.00	0.00	H
ATOM	351	N	GLU	146	8.791	14.004	23.712	1.00	0.00	N
ATOM	352	CA	GLU	146	7.727	13.932	24.661	1.00	0.00	C
ATOM	353	C	GLU	146	7.460	15.289	25.248	1.00	0.00	C
ATOM	354	O	GLU	146	6.301	15.676	25.417	1.00	0.00	O
ATOM	355	CB	GLU	146	7.955	12.919	25.785	1.00	0.00	C
ATOM	356	CG	GLU	146	6.927	13.058	26.897	1.00	0.00	C
ATOM	357	CD	GLU	146	5.522	12.785	26.372	1.00	0.00	C
ATOM	358	OE1	GLU	146	5.141	13.300	25.282	1.00	0.00	O
ATOM	359	OE2	GLU	146	4.797	12.056	27.087	1.00	0.00	O
ATOM	360	H	GLU	146	9.670	13.485	23.844	1.00	0.00	H
ATOM	361	HA	GLU	146	6.816	13.574	24.180	1.00	0.00	H
ATOM	362	1HB	GLU	146	8.935	13.033	26.247	1.00	0.00	H
ATOM	363	2HB	GLU	146	7.894	11.890	25.428	1.00	0.00	H
ATOM	364	1HG	GLU	146	6.943	14.064	27.315	1.00	0.00	H
ATOM	365	2HG	GLU	146	7.131	12.352	27.702	1.00	0.00	H
ATOM	366	N	PHE	147	8.519	16.052	25.589	1.00	0.00	N
ATOM	367	CA	PHE	147	8.267	17.365	26.115	1.00	0.00	C
ATOM	368	C	PHE	147	7.670	18.299	25.118	1.00	0.00	C
ATOM	369	O	PHE	147	6.691	18.985	25.413	1.00	0.00	O
ATOM	370	CB	PHE	147	9.479	18.072	26.751	1.00	0.00	C
ATOM	371	CG	PHE	147	9.295	17.919	28.217	1.00	0.00	C
ATOM	372	CD1	PHE	147	9.728	16.820	28.917	1.00	0.00	C
ATOM	373	CD2	PHE	147	8.621	18.916	28.880	1.00	0.00	C
ATOM	374	CE1	PHE	147	9.500	16.753	30.273	1.00	0.00	C
ATOM	375	CE2	PHE	147	8.396	18.852	30.231	1.00	0.00	C
ATOM	376	CZ	PHE	147	8.844	17.762	30.935	1.00	0.00	C
ATOM	377	H	PHE	147	9.481	15.703	25.475	1.00	0.00	H
ATOM	378	HA	PHE	147	7.577	17.369	26.959	1.00	0.00	H
ATOM	379	1HB	PHE	147	9.416	19.106	26.413	1.00	0.00	H
ATOM	380	2HB	PHE	147	10.352	17.544	26.367	1.00	0.00	H
ATOM	381	HD1	PHE	147	10.246	16.009	28.404	1.00	0.00	H
ATOM	382	HD2	PHE	147	8.257	19.777	28.319	1.00	0.00	H
ATOM	383	HE1	PHE	147	9.846	15.883	30.831	1.00	0.00	H
ATOM	384	HE2	PHE	147	7.867	19.657	30.740	1.00	0.00	H
ATOM	385	HZ	PHE	147	8.680	17.697	32.010	1.00	0.00	H
ATOM	386	N	LEU	148	8.228	18.345	23.901	1.00	0.00	N
ATOM	387	CA	LEU	148	7.756	19.335	22.986	1.00	0.00	C
ATOM	388	C	LEU	148	6.317	19.106	22.646	1.00	0.00	C
ATOM	389	O	LEU	148	5.555	20.070	22.555	1.00	0.00	O
ATOM	390	CB	LEU	148	8.611	19.432	21.719	1.00	0.00	C
ATOM	391	CG	LEU	148	10.027	19.958	22.036	1.00	0.00	C
ATOM	392	CD1	LEU	148	10.877	20.091	20.763	1.00	0.00	C
ATOM	393	CD2	LEU	148	9.967	21.255	22.861	1.00	0.00	C
ATOM	394	H	LEU	148	8.974	17.687	23.633	1.00	0.00	H
ATOM	395	HA	LEU	148	7.845	20.334	23.412	1.00	0.00	H
ATOM	396	1HB	LEU	148	8.164	20.108	20.990	1.00	0.00	H
ATOM	397	2HB	LEU	148	8.721	18.459	21.239	1.00	0.00	H
ATOM	398	HG	LEU	148	10.559	19.290	22.713	1.00	0.00	H
ATOM	399	1HD1	LEU	148	10.289	19.781	19.899	1.00	0.00	H
ATOM	400	2HD1	LEU	148	11.185	21.128	20.638	1.00	0.00	H
ATOM	401	3HD1	LEU	148	11.759	19.457	20.847	1.00	0.00	H
ATOM	402	1HD2	LEU	148	8.926	21.522	23.043	1.00	0.00	H
ATOM	403	2HD2	LEU	148	10.475	21.104	23.813	1.00	0.00	H

ATOM	404	3HD2	LEU	148	10.457	22.058	22.311	1.00	0.00	H
ATOM	405	N	THR	149	5.881	17.845	22.464	1.00	0.00	N
ATOM	406	CA	THR	149	4.505	17.686	22.089	1.00	0.00	C
ATOM	407	C	THR	149	3.639	17.773	23.311	1.00	0.00	C
ATOM	408	O	THR	149	2.939	16.829	23.673	1.00	0.00	O
ATOM	409	CB	THR	149	4.203	16.400	21.368	1.00	0.00	C
ATOM	410	OG1	THR	149	4.989	16.316	20.188	1.00	0.00	O
ATOM	411	CG2	THR	149	2.711	16.386	20.982	1.00	0.00	C
ATOM	412	H	THR	149	6.504	17.034	22.587	1.00	0.00	H
ATOM	413	HA	THR	149	4.224	18.473	21.389	1.00	0.00	H
ATOM	414	HB	THR	149	4.427	15.564	22.031	1.00	0.00	H
ATOM	415	HG1	THR	149	5.121	17.259	19.795	1.00	0.00	H
ATOM	416	1HG2	THR	149	2.238	17.306	21.323	1.00	0.00	H
ATOM	417	2HG2	THR	149	2.616	16.309	19.898	1.00	0.00	H
ATOM	418	3HG2	THR	149	2.222	15.531	21.450	1.00	0.00	H
ATOM	419	N	SER	150	3.672	18.934	23.987	1.00	0.00	N
ATOM	420	CA	SER	150	2.792	19.149	25.095	1.00	0.00	C
ATOM	421	C	SER	150	1.441	19.352	24.478	1.00	0.00	C
ATOM	422	O	SER	150	1.340	19.828	23.350	1.00	0.00	O
ATOM	423	CB	SER	150	3.136	20.402	25.916	1.00	0.00	C
ATOM	424	OG	SER	150	2.239	20.543	27.008	1.00	0.00	O
ATOM	425	H	SER	150	4.333	19.672	23.706	1.00	0.00	H
ATOM	426	HA	SER	150	2.868	18.240	25.692	1.00	0.00	H
ATOM	427	1HB	SER	150	3.066	21.295	25.295	1.00	0.00	H
ATOM	428	2HB	SER	150	4.150	20.333	26.309	1.00	0.00	H
ATOM	429	HG	SER	150	2.118	21.542	27.226	1.00	0.00	H
ATOM	430	N	ALA	151	0.353	18.994	25.191	1.00	0.00	N
ATOM	431	CA	ALA	151	-0.938	19.093	24.579	1.00	0.00	C
ATOM	432	C	ALA	151	-1.199	20.514	24.215	1.00	0.00	C
ATOM	433	O	ALA	151	-1.451	20.805	23.050	1.00	0.00	O
ATOM	434	CB	ALA	151	-2.081	18.634	25.500	1.00	0.00	C
ATOM	435	H	ALA	151	0.449	18.655	26.158	1.00	0.00	H
ATOM	436	HA	ALA	151	-0.957	18.473	23.682	1.00	0.00	H
ATOM	437	1HB	ALA	151	-1.670	18.316	26.458	1.00	0.00	H
ATOM	438	2HB	ALA	151	-2.775	19.459	25.657	1.00	0.00	H
ATOM	439	3HB	ALA	151	-2.608	17.799	25.037	1.00	0.00	H
ATOM	440	N	ASN	152	-1.074	21.419	25.208	1.00	0.00	N
ATOM	441	CA	ASN	152	-1.299	22.839	25.124	1.00	0.00	C
ATOM	442	C	ASN	152	-2.555	23.137	25.881	1.00	0.00	C
ATOM	443	O	ASN	152	-2.645	24.149	26.571	1.00	0.00	O
ATOM	444	CB	ASN	152	-1.443	23.453	23.706	1.00	0.00	C
ATOM	445	CG	ASN	152	-2.843	23.286	23.104	1.00	0.00	C
ATOM	446	OD1	ASN	152	-3.517	22.258	23.159	1.00	0.00	O
ATOM	447	ND2	ASN	152	-3.313	24.403	22.485	1.00	0.00	N
ATOM	448	H	ASN	152	-0.786	21.054	26.127	1.00	0.00	H
ATOM	449	HA	ASN	152	-0.435	23.331	25.571	1.00	0.00	H
ATOM	450	1HB	ASN	152	-0.765	23.018	22.971	1.00	0.00	H
ATOM	451	2HB	ASN	152	-1.246	24.524	23.672	1.00	0.00	H
ATOM	452	1HD2	ASN	152	-4.247	24.397	22.052	1.00	0.00	H
ATOM	453	2HD2	ASN	152	-2.734	25.254	22.449	1.00	0.00	H
ATOM	454	N	LYS	153	-3.577	22.269	25.770	1.00	0.00	N
ATOM	455	CA	LYS	153	-4.751	22.505	26.551	1.00	0.00	C
ATOM	456	C	LYS	153	-4.348	22.302	27.967	1.00	0.00	C
ATOM	457	O	LYS	153	-4.538	23.175	28.813	1.00	0.00	O
ATOM	458	CB	LYS	153	-5.884	21.508	26.258	1.00	0.00	C
ATOM	459	CG	LYS	153	-6.668	21.807	24.979	1.00	0.00	C
ATOM	460	CD	LYS	153	-7.456	23.119	25.040	1.00	0.00	C
ATOM	461	CE	LYS	153	-8.706	23.049	25.924	1.00	0.00	C
ATOM	462	NZ	LYS	153	-9.731	22.186	25.293	1.00	0.00	N
ATOM	463	H	LYS	153	-3.515	21.456	25.139	1.00	0.00	H
ATOM	464	HA	LYS	153	-5.049	23.532	26.341	1.00	0.00	H
ATOM	465	1HB	LYS	153	-6.586	21.533	27.090	1.00	0.00	H
ATOM	466	2HB	LYS	153	-5.447	20.514	26.154	1.00	0.00	H
ATOM	467	1HG	LYS	153	-7.404	21.042	24.733	1.00	0.00	H
ATOM	468	2HG	LYS	153	-6.037	21.892	24.094	1.00	0.00	H
ATOM	469	1HD	LYS	153	-7.819	23.459	24.070	1.00	0.00	H
ATOM	470	2HD	LYS	153	-6.882	23.958	25.433	1.00	0.00	H
ATOM	471	1HE	LYS	153	-9.125	24.045	26.063	1.00	0.00	H

ATOM	472	2HE	LYS	153	-8.453	22.635	26.900	1.00	0.00	H
ATOM	473	1HZ	LYS	153	-9.372	21.824	24.397	1.00	0.00	H
ATOM	474	2HZ	LYS	153	-9.948	21.397	25.918	1.00	0.00	H
ATOM	475	3HZ	LYS	153	-10.585	22.735	25.123	1.00	0.00	H
ATOM	476	N	HIS	154	-3.749	21.128	28.244	1.00	0.00	N
ATOM	477	CA	HIS	154	-3.330	20.820	29.574	1.00	0.00	C
ATOM	478	C	HIS	154	-2.229	21.764	29.916	1.00	0.00	C
ATOM	479	O	HIS	154	-2.313	22.481	30.912	1.00	0.00	O
ATOM	480	CB	HIS	154	-2.854	19.366	29.707	1.00	0.00	C
ATOM	481	CG	HIS	154	-3.979	18.411	29.430	1.00	0.00	C
ATOM	482	ND1	HIS	154	-3.823	17.066	29.176	1.00	0.00	N
ATOM	483	CD2	HIS	154	-5.318	18.647	29.367	1.00	0.00	C
ATOM	484	CE1	HIS	154	-5.066	16.560	28.973	1.00	0.00	C
ATOM	485	NE2	HIS	154	-6.006	17.482	29.079	1.00	0.00	N
ATOM	486	H	HIS	154	-3.591	20.445	27.488	1.00	0.00	H
ATOM	487	HA	HIS	154	-4.195	20.957	30.222	1.00	0.00	H
ATOM	488	1HB	HIS	154	-2.483	19.171	30.713	1.00	0.00	H
ATOM	489	2HB	HIS	154	-2.049	19.157	29.001	1.00	0.00	H
ATOM	490	HD1	HIS	154	-2.934	16.545	29.146	1.00	0.00	H
ATOM	491	HD2	HIS	154	-5.784	19.620	29.522	1.00	0.00	H
ATOM	492	HE1	HIS	154	-5.265	15.512	28.748	1.00	0.00	H
ATOM	493	HE2	HIS	154	-7.023	17.360	28.971	1.00	0.00	H
ATOM	494	N	PHE	155	-1.165	21.818	29.089	1.00	0.00	N
ATOM	495	CA	PHE	155	-0.190	22.815	29.405	1.00	0.00	C
ATOM	496	C	PHE	155	-0.650	23.984	28.609	1.00	0.00	C
ATOM	497	O	PHE	155	-0.273	24.133	27.448	1.00	0.00	O
ATOM	498	CB	PHE	155	1.245	22.479	28.971	1.00	0.00	C
ATOM	499	CG	PHE	155	2.127	23.357	29.793	1.00	0.00	C
ATOM	500	CD1	PHE	155	2.314	24.682	29.487	1.00	0.00	C
ATOM	501	CD2	PHE	155	2.767	22.844	30.895	1.00	0.00	C
ATOM	502	CE1	PHE	155	3.128	25.474	30.263	1.00	0.00	C
ATOM	503	CE2	PHE	155	3.583	23.629	31.675	1.00	0.00	C
ATOM	504	CZ	PHE	155	3.767	24.952	31.359	1.00	0.00	C
ATOM	505	H	PHE	155	-1.061	21.183	28.284	1.00	0.00	H
ATOM	506	HA	PHE	155	-0.175	23.027	30.474	1.00	0.00	H
ATOM	507	1HB	PHE	155	1.288	22.706	27.905	1.00	0.00	H
ATOM	508	2HB	PHE	155	1.375	21.418	29.188	1.00	0.00	H
ATOM	509	HD1	PHE	155	1.812	25.111	28.619	1.00	0.00	H
ATOM	510	HD2	PHE	155	2.625	21.795	31.155	1.00	0.00	H
ATOM	511	HE1	PHE	155	3.266	26.524	30.005	1.00	0.00	H
ATOM	512	HE2	PHE	155	4.083	23.201	32.543	1.00	0.00	H
ATOM	513	HZ	PHE	155	4.413	25.580	31.971	1.00	0.00	H
ATOM	514	N	MET	156	-1.446	24.859	29.262	1.00	0.00	N
ATOM	515	CA	MET	156	-2.169	25.915	28.617	1.00	0.00	C
ATOM	516	C	MET	156	-1.274	26.681	27.710	1.00	0.00	C
ATOM	517	O	MET	156	-1.482	26.694	26.498	1.00	0.00	O
ATOM	518	CB	MET	156	-2.778	26.915	29.617	1.00	0.00	C
ATOM	519	CG	MET	156	-3.719	27.936	28.973	1.00	0.00	C
ATOM	520	SD	MET	156	-5.305	27.249	28.409	1.00	0.00	S
ATOM	521	CE	MET	156	-5.925	26.894	30.079	1.00	0.00	C
ATOM	522	H	MET	156	-1.538	24.761	30.283	1.00	0.00	H
ATOM	523	HA	MET	156	-2.991	25.510	28.027	1.00	0.00	H
ATOM	524	1HB	MET	156	-2.036	27.513	30.146	1.00	0.00	H
ATOM	525	2HB	MET	156	-3.370	26.445	30.402	1.00	0.00	H
ATOM	526	1HG	MET	156	-3.217	28.362	28.104	1.00	0.00	H
ATOM	527	2HG	MET	156	-3.938	28.709	29.708	1.00	0.00	H
ATOM	528	1HE	MET	156	-5.179	27.195	30.815	1.00	0.00	H
ATOM	529	2HE	MET	156	-6.848	27.447	30.249	1.00	0.00	H
ATOM	530	3HE	MET	156	-6.119	25.825	30.175	1.00	0.00	H
ATOM	531	N	VAL	157	-0.237	27.331	28.256	1.00	0.00	N
ATOM	532	CA	VAL	157	0.589	28.078	27.364	1.00	0.00	C
ATOM	533	C	VAL	157	1.258	27.091	26.474	1.00	0.00	C
ATOM	534	O	VAL	157	1.390	27.309	25.271	1.00	0.00	O
ATOM	535	CB	VAL	157	1.637	28.902	28.060	1.00	0.00	C
ATOM	536	CG1	VAL	157	2.615	27.972	28.791	1.00	0.00	C
ATOM	537	CG2	VAL	157	2.316	29.803	27.016	1.00	0.00	C
ATOM	538	H	VAL	157	-0.046	27.293	29.267	1.00	0.00	H
ATOM	539	HA	VAL	157	-0.071	28.746	26.812	1.00	0.00	H

ATOM	540	HB	VAL	157	1.157	29.565	28.780	1.00	0.00	H
ATOM	541	1HG1	VAL	157	2.318	26.935	28.632	1.00	0.00	H
ATOM	542	2HG1	VAL	157	3.621	28.124	28.402	1.00	0.00	H
ATOM	543	3HG1	VAL	157	2.600	28.194	29.857	1.00	0.00	H
ATOM	544	1HG2	VAL	157	1.872	29.622	26.036	1.00	0.00	H
ATOM	545	2HG2	VAL	157	2.175	30.848	27.291	1.00	0.00	H
ATOM	546	3HG2	VAL	157	3.381	29.577	26.979	1.00	0.00	H
ATOM	547	N	GLY	158	1.682	25.952	27.051	1.00	0.00	N
ATOM	548	CA	GLY	158	2.374	24.964	26.287	1.00	0.00	C
ATOM	549	C	GLY	158	3.693	25.566	25.964	1.00	0.00	C
ATOM	550	O	GLY	158	4.422	25.074	25.105	1.00	0.00	O
ATOM	551	H	GLY	158	1.505	25.791	28.053	1.00	0.00	H
ATOM	552	1HA	GLY	158	1.754	24.790	25.407	1.00	0.00	H
ATOM	553	2HA	GLY	158	2.447	24.092	26.938	1.00	0.00	H
ATOM	554	N	HIS	159	4.039	26.665	26.659	1.00	0.00	N
ATOM	555	CA	HIS	159	5.280	27.303	26.363	1.00	0.00	C
ATOM	556	C	HIS	159	6.185	27.184	27.537	1.00	0.00	C
ATOM	557	O	HIS	159	6.237	28.065	28.394	1.00	0.00	O
ATOM	558	CB	HIS	159	5.130	28.805	26.067	1.00	0.00	C
ATOM	559	CG	HIS	159	6.430	29.485	25.748	1.00	0.00	C
ATOM	560	ND1	HIS	159	7.012	29.494	24.501	1.00	0.00	N
ATOM	561	CD2	HIS	159	7.268	30.197	26.553	1.00	0.00	C
ATOM	562	CE1	HIS	159	8.162	30.205	24.609	1.00	0.00	C
ATOM	563	NE2	HIS	159	8.361	30.653	25.836	1.00	0.00	N
ATOM	564	H	HIS	159	3.418	27.038	27.391	1.00	0.00	H
ATOM	565	HA	HIS	159	5.735	26.820	25.498	1.00	0.00	H
ATOM	566	1HB	HIS	159	4.708	29.371	26.897	1.00	0.00	H
ATOM	567	2HB	HIS	159	4.481	29.017	25.217	1.00	0.00	H
ATOM	568	HD1	HIS	159	6.644	29.046	23.649	1.00	0.00	H
ATOM	569	HD2	HIS	159	7.100	30.381	27.614	1.00	0.00	H
ATOM	570	HE1	HIS	159	8.844	30.386	23.778	1.00	0.00	H
ATOM	571	HE2	HIS	159	9.151	31.215	26.181	1.00	0.00	H
ATOM	572	N	PRO	160	6.878	26.091	27.621	1.00	0.00	N
ATOM	573	CA	PRO	160	7.881	25.999	28.636	1.00	0.00	C
ATOM	574	C	PRO	160	9.130	26.444	27.957	1.00	0.00	C
ATOM	575	O	PRO	160	9.143	26.496	26.728	1.00	0.00	O
ATOM	576	CB	PRO	160	7.936	24.532	29.067	1.00	0.00	C
ATOM	577	CG	PRO	160	7.240	23.770	27.930	1.00	0.00	C
ATOM	578	CD	PRO	160	6.260	24.803	27.361	1.00	0.00	C
ATOM	579	HA	PRO	160	7.532	26.674	29.417	1.00	0.00	H
ATOM	580	1HB	PRO	160	7.395	24.504	30.013	1.00	0.00	H
ATOM	581	2HB	PRO	160	8.999	24.313	29.159	1.00	0.00	H
ATOM	582	1HG	PRO	160	6.723	22.887	28.308	1.00	0.00	H
ATOM	583	2HG	PRO	160	7.960	23.440	27.181	1.00	0.00	H
ATOM	584	1HD	PRO	160	6.156	24.753	26.277	1.00	0.00	H
ATOM	585	2HD	PRO	160	5.306	24.835	27.888	1.00	0.00	H
ATOM	586	N	VAL	161	10.179	26.798	28.715	1.00	0.00	N
ATOM	587	CA	VAL	161	11.414	27.057	28.050	1.00	0.00	C
ATOM	588	C	VAL	161	12.184	25.811	28.276	1.00	0.00	C
ATOM	589	O	VAL	161	12.576	25.516	29.404	1.00	0.00	O
ATOM	590	CB	VAL	161	12.211	28.183	28.640	1.00	0.00	C
ATOM	591	CG1	VAL	161	13.571	28.240	27.924	1.00	0.00	C
ATOM	592	CG2	VAL	161	11.394	29.479	28.519	1.00	0.00	C
ATOM	593	H	VAL	161	10.095	26.879	29.738	1.00	0.00	H
ATOM	594	HA	VAL	161	11.255	27.250	26.989	1.00	0.00	H
ATOM	595	HB	VAL	161	12.345	27.987	29.703	1.00	0.00	H
ATOM	596	1HG1	VAL	161	13.618	27.453	27.170	1.00	0.00	H
ATOM	597	2HG1	VAL	161	13.688	29.211	27.443	1.00	0.00	H
ATOM	598	3HG1	VAL	161	14.370	28.095	28.650	1.00	0.00	H
ATOM	599	1HG2	VAL	161	10.440	29.264	28.036	1.00	0.00	H
ATOM	600	2HG2	VAL	161	11.213	29.889	29.512	1.00	0.00	H
ATOM	601	3HG2	VAL	161	11.947	30.203	27.921	1.00	0.00	H
ATOM	602	N	ILE	162	12.401	25.022	27.213	1.00	0.00	N
ATOM	603	CA	ILE	162	13.098	23.805	27.455	1.00	0.00	C
ATOM	604	C	ILE	162	14.534	24.031	27.149	1.00	0.00	C
ATOM	605	O	ILE	162	14.913	24.289	26.011	1.00	0.00	O
ATOM	606	CB	ILE	162	12.561	22.641	26.660	1.00	0.00	C
ATOM	607	CG1	ILE	162	13.202	21.326	27.125	1.00	0.00	C

```
ATOM    608  CG2 ILE   162      12.704  22.921  25.157  1.00  0.00           C
ATOM    609  CD1 ILE   162      12.483  20.090  26.587  1.00  0.00           C
ATOM    610  H   ILE   162      12.079  25.283  26.270  1.00  0.00           H
ATOM    611  HA  ILE   162      12.959  23.541  28.503  1.00  0.00           H
ATOM    612  HB  ILE   162      11.507  22.485  26.892  1.00  0.00           H
ATOM    613 1HG1 ILE   162      13.208  21.216  28.209  1.00  0.00           H
ATOM    614 2HG1 ILE   162      14.240  21.225  26.810  1.00  0.00           H
ATOM    615 1HG2 ILE   162      13.162  23.899  25.011  1.00  0.00           H
ATOM    616 2HG2 ILE   162      13.332  22.154  24.702  1.00  0.00           H
ATOM    617 3HG2 ILE   162      11.719  22.907  24.689  1.00  0.00           H
ATOM    618 1HD1 ILE   162      11.641  20.399  25.967  1.00  0.00           H
ATOM    619 2HD1 ILE   162      13.175  19.498  25.988  1.00  0.00           H
ATOM    620 3HD1 ILE   162      12.118  19.489  27.420  1.00  0.00           H
ATOM    621  N   PHE   163      15.381  23.965  28.191  1.00  0.00           N
ATOM    622  CA  PHE   163      16.786  24.084  27.985  1.00  0.00           C
ATOM    623  C   PHE   163      17.125  22.659  27.726  1.00  0.00           C
ATOM    624  O   PHE   163      17.897  22.033  28.449  1.00  0.00           O
ATOM    625  CB  PHE   163      17.495  24.524  29.276  1.00  0.00           C
ATOM    626  CG  PHE   163      18.695  25.330  28.926  1.00  0.00           C
ATOM    627  CD1 PHE   163      19.891  24.765  28.556  1.00  0.00           C
ATOM    628  CD2 PHE   163      18.592  26.700  28.988  1.00  0.00           C
ATOM    629  CE1 PHE   163      20.963  25.573  28.249  1.00  0.00           C
ATOM    630  CE2 PHE   163      19.659  27.508  28.683  1.00  0.00           C
ATOM    631  CZ  PHE   163      20.852  26.942  28.311  1.00  0.00           C
ATOM    632  H   PHE   163      15.012  23.827  29.143  1.00  0.00           H
ATOM    633  HA  PHE   163      17.020  24.740  27.146  1.00  0.00           H
ATOM    634 1HB  PHE   163      17.797  23.640  29.838  1.00  0.00           H
ATOM    635 2HB  PHE   163      16.810  25.125  29.874  1.00  0.00           H
ATOM    636  HD1 PHE   163      19.991  23.680  28.505  1.00  0.00           H
ATOM    637  HD2 PHE   163      17.645  27.152  29.284  1.00  0.00           H
ATOM    638  HE1 PHE   163      21.910  25.122  27.953  1.00  0.00           H
ATOM    639  HE2 PHE   163      19.559  28.592  28.736  1.00  0.00           H
ATOM    640  HZ  PHE   163      21.706  27.573  28.066  1.00  0.00           H
ATOM    641  N   TYR   164      16.533  22.115  26.649  1.00  0.00           N
ATOM    642  CA  TYR   164      16.658  20.723  26.383  1.00  0.00           C
ATOM    643  C   TYR   164      18.087  20.449  26.152  1.00  0.00           C
ATOM    644  O   TYR   164      18.573  19.357  26.444  1.00  0.00           O
ATOM    645  CB  TYR   164      15.861  20.235  25.146  1.00  0.00           C
ATOM    646  CG  TYR   164      16.389  20.821  23.873  1.00  0.00           C
ATOM    647  CD1 TYR   164      17.522  20.314  23.271  1.00  0.00           C
ATOM    648  CD2 TYR   164      15.731  21.861  23.256  1.00  0.00           C
ATOM    649  CE1 TYR   164      18.005  20.845  22.098  1.00  0.00           C
ATOM    650  CE2 TYR   164      16.207  22.397  22.081  1.00  0.00           C
ATOM    651  CZ  TYR   164      17.347  21.893  21.500  1.00  0.00           C
ATOM    652  OH  TYR   164      17.836  22.443  20.297  1.00  0.00           O
ATOM    653  H   TYR   164      15.984  22.710  26.011  1.00  0.00           H
ATOM    654  HA  TYR   164      16.284  20.191  27.258  1.00  0.00           H
ATOM    655 1HB  TYR   164      14.807  20.507  25.206  1.00  0.00           H
ATOM    656 2HB  TYR   164      15.901  19.151  25.036  1.00  0.00           H
ATOM    657  HD1 TYR   164      18.044  19.476  23.733  1.00  0.00           H
ATOM    658  HD2 TYR   164      14.822  22.264  23.703  1.00  0.00           H
ATOM    659  HE1 TYR   164      18.907  20.435  21.643  1.00  0.00           H
ATOM    660  HE2 TYR   164      15.677  23.224  21.608  1.00  0.00           H
ATOM    661  HH  TYR   164      18.333  23.321  20.498  1.00  0.00           H
ATOM    662  N   ILE   165      18.824  21.440  25.631  1.00  0.00           N
ATOM    663  CA  ILE   165      20.121  20.985  25.289  1.00  0.00           C
ATOM    664  C   ILE   165      21.181  21.517  26.199  1.00  0.00           C
ATOM    665  O   ILE   165      21.709  22.613  26.027  1.00  0.00           O
ATOM    666  CB  ILE   165      20.447  21.230  23.830  1.00  0.00           C
ATOM    667  CG1 ILE   165      21.665  20.408  23.365  1.00  0.00           C
ATOM    668  CG2 ILE   165      20.533  22.742  23.568  1.00  0.00           C
ATOM    669  CD1 ILE   165      22.997  20.777  24.012  1.00  0.00           C
ATOM    670  H   ILE   165      18.491  22.405  25.497  1.00  0.00           H
ATOM    671  HA  ILE   165      20.212  19.899  25.326  1.00  0.00           H
ATOM    672  HB  ILE   165      19.666  20.798  23.203  1.00  0.00           H
ATOM    673 1HG1 ILE   165      21.778  20.553  22.290  1.00  0.00           H
ATOM    674 2HG1 ILE   165      21.472  19.360  23.598  1.00  0.00           H
ATOM    675 1HG2 ILE   165      20.339  23.283  24.494  1.00  0.00           H
```

ATOM	676	2HG2	ILE	165	21.529	22.992	23.203	1.00	0.00	H
ATOM	677	3HG2	ILE	165	19.791	23.024	22.820	1.00	0.00	H
ATOM	678	1HD1	ILE	165	22.844	21.592	24.719	1.00	0.00	H
ATOM	679	2HD1	ILE	165	23.398	19.910	24.537	1.00	0.00	H
ATOM	680	3HD1	ILE	165	23.700	21.092	23.241	1.00	0.00	H
ATOM	681	N	MET	166	21.499	20.724	27.236	1.00	0.00	N
ATOM	682	CA	MET	166	22.695	20.976	27.973	1.00	0.00	C
ATOM	683	C	MET	166	23.516	19.802	27.587	1.00	0.00	C
ATOM	684	O	MET	166	23.480	18.760	28.239	1.00	0.00	O
ATOM	685	CB	MET	166	22.531	20.969	29.497	1.00	0.00	C
ATOM	686	CG	MET	166	21.894	22.253	30.014	1.00	0.00	C
ATOM	687	SD	MET	166	22.909	23.743	29.768	1.00	0.00	S
ATOM	688	CE	MET	166	24.234	23.246	30.907	1.00	0.00	C
ATOM	689	H	MET	166	20.884	19.940	27.497	1.00	0.00	H
ATOM	690	HA	MET	166	23.152	21.922	27.685	1.00	0.00	H
ATOM	691	1HB	MET	166	23.485	20.865	30.013	1.00	0.00	H
ATOM	692	2HB	MET	166	21.900	20.148	29.840	1.00	0.00	H
ATOM	693	1HG	MET	166	21.721	22.142	31.084	1.00	0.00	H
ATOM	694	2HG	MET	166	20.951	22.403	29.487	1.00	0.00	H
ATOM	695	1HE	MET	166	23.997	22.273	31.338	1.00	0.00	H
ATOM	696	2HE	MET	166	25.176	23.182	30.363	1.00	0.00	H
ATOM	697	3HE	MET	166	24.324	23.983	31.704	1.00	0.00	H
ATOM	698	N	VAL	167	24.282	19.947	26.494	1.00	0.00	N
ATOM	699	CA	VAL	167	24.972	18.801	25.997	1.00	0.00	C
ATOM	700	C	VAL	167	26.352	18.808	26.540	1.00	0.00	C
ATOM	701	O	VAL	167	26.993	19.851	26.660	1.00	0.00	O
ATOM	702	CB	VAL	167	25.078	18.751	24.502	1.00	0.00	C
ATOM	703	CG1	VAL	167	26.003	19.894	24.048	1.00	0.00	C
ATOM	704	CG2	VAL	167	25.571	17.354	24.093	1.00	0.00	C
ATOM	705	H	VAL	167	24.369	20.860	26.026	1.00	0.00	H
ATOM	706	HA	VAL	167	24.440	17.907	26.323	1.00	0.00	H
ATOM	707	HB	VAL	167	24.078	18.875	24.086	1.00	0.00	H
ATOM	708	1HG1	VAL	167	26.348	20.450	24.919	1.00	0.00	H
ATOM	709	2HG1	VAL	167	26.861	19.479	23.519	1.00	0.00	H
ATOM	710	3HG1	VAL	167	25.455	20.562	23.383	1.00	0.00	H
ATOM	711	1HG2	VAL	167	25.721	16.745	24.984	1.00	0.00	H
ATOM	712	2HG2	VAL	167	24.828	16.879	23.451	1.00	0.00	H
ATOM	713	3HG2	VAL	167	26.513	17.444	23.552	1.00	0.00	H
ATOM	714	N	ASP	168	26.836	17.613	26.917	1.00	0.00	N
ATOM	715	CA	ASP	168	28.165	17.525	27.426	1.00	0.00	C
ATOM	716	C	ASP	168	29.058	17.306	26.251	1.00	0.00	C
ATOM	717	O	ASP	168	29.868	16.381	26.249	1.00	0.00	O
ATOM	718	CB	ASP	168	28.387	16.336	28.371	1.00	0.00	C
ATOM	719	CG	ASP	168	29.851	15.945	28.259	1.00	0.00	C
ATOM	720	OD1	ASP	168	30.612	16.679	27.573	1.00	0.00	O
ATOM	721	OD2	ASP	168	30.235	14.914	28.870	1.00	0.00	O
ATOM	722	H	ASP	168	26.252	16.767	26.839	1.00	0.00	H
ATOM	723	HA	ASP	168	28.369	18.470	27.927	1.00	0.00	H
ATOM	724	1HB	ASP	168	27.728	15.536	28.038	1.00	0.00	H
ATOM	725	2HB	ASP	168	28.136	16.676	29.377	1.00	0.00	H
ATOM	726	N	ASP	169	28.943	18.184	25.234	1.00	0.00	N
ATOM	727	CA	ASP	169	29.722	18.092	24.032	1.00	0.00	C
ATOM	728	C	ASP	169	29.683	16.694	23.501	1.00	0.00	C
ATOM	729	O	ASP	169	30.666	15.958	23.583	1.00	0.00	O
ATOM	730	CB	ASP	169	31.194	18.496	24.209	1.00	0.00	C
ATOM	731	CG	ASP	169	32.052	17.421	23.556	1.00	0.00	C
ATOM	732	OD1	ASP	169	32.403	17.591	22.357	1.00	0.00	O
ATOM	733	OD2	ASP	169	32.363	16.413	24.244	1.00	0.00	O
ATOM	734	H	ASP	169	28.266	18.955	25.323	1.00	0.00	H
ATOM	735	HA	ASP	169	29.323	18.767	23.275	1.00	0.00	H
ATOM	736	1HB	ASP	169	31.393	18.562	25.278	1.00	0.00	H
ATOM	737	2HB	ASP	169	31.334	19.460	23.722	1.00	0.00	H
ATOM	738	N	VAL	170	28.531	16.285	22.936	1.00	0.00	N
ATOM	739	CA	VAL	170	28.426	14.963	22.396	1.00	0.00	C
ATOM	740	C	VAL	170	28.652	15.052	20.924	1.00	0.00	C
ATOM	741	O	VAL	170	28.473	16.106	20.317	1.00	0.00	O
ATOM	742	CB	VAL	170	27.084	14.333	22.627	1.00	0.00	C
ATOM	743	CG1	VAL	170	27.074	12.924	22.011	1.00	0.00	C

ATOM	744	CG2	VAL	170	26.794	14.357	24.139	1.00	0.00	C
ATOM	745	H	VAL	170	27.724	16.924	22.892	1.00	0.00	H
ATOM	746	HA	VAL	170	29.187	14.346	22.873	1.00	0.00	H
ATOM	747	HB	VAL	170	26.314	14.945	22.157	1.00	0.00	H
ATOM	748	1HG1	VAL	170	28.042	12.719	21.554	1.00	0.00	H
ATOM	749	2HG1	VAL	170	26.877	12.187	22.790	1.00	0.00	H
ATOM	750	3HG1	VAL	170	26.294	12.864	21.251	1.00	0.00	H
ATOM	751	1HG2	VAL	170	27.629	14.822	24.662	1.00	0.00	H
ATOM	752	2HG2	VAL	170	25.885	14.928	24.326	1.00	0.00	H
ATOM	753	3HG2	VAL	170	26.662	13.337	24.500	1.00	0.00	H
ATOM	754	N	SER	171	29.090	13.940	20.310	1.00	0.00	N
ATOM	755	CA	SER	171	29.316	13.919	18.897	1.00	0.00	C
ATOM	756	C	SER	171	27.985	13.651	18.275	1.00	0.00	C
ATOM	757	O	SER	171	26.978	13.649	18.980	1.00	0.00	O
ATOM	758	CB	SER	171	30.306	12.816	18.459	1.00	0.00	C
ATOM	759	OG	SER	171	30.577	12.901	17.067	1.00	0.00	O
ATOM	760	H	SER	171	29.265	13.090	20.864	1.00	0.00	H
ATOM	761	HA	SER	171	29.710	14.903	18.644	1.00	0.00	H
ATOM	762	1HB	SER	171	29.900	11.825	18.662	1.00	0.00	H
ATOM	763	2HB	SER	171	31.252	12.908	18.992	1.00	0.00	H
ATOM	764	HG	SER	171	30.700	13.888	16.800	1.00	0.00	H
ATOM	765	N	ARG	172	27.978	13.425	16.942	1.00	0.00	N
ATOM	766	CA	ARG	172	26.839	13.151	16.103	1.00	0.00	C
ATOM	767	C	ARG	172	25.594	13.778	16.650	1.00	0.00	C
ATOM	768	O	ARG	172	24.658	13.096	17.058	1.00	0.00	O
ATOM	769	CB	ARG	172	26.582	11.647	15.910	1.00	0.00	C
ATOM	770	CG	ARG	172	25.412	11.334	14.976	1.00	0.00	C
ATOM	771	CD	ARG	172	25.168	9.834	14.794	1.00	0.00	C
ATOM	772	NE	ARG	172	24.011	9.670	13.869	1.00	0.00	N
ATOM	773	CZ	ARG	172	23.678	8.427	13.414	1.00	0.00	C
ATOM	774	NH1	ARG	172	24.396	7.338	13.815	1.00	0.00	N
ATOM	775	NH2	ARG	172	22.625	8.271	12.560	1.00	0.00	N
ATOM	776	H	ARG	172	28.893	13.451	16.471	1.00	0.00	H
ATOM	777	HA	ARG	172	26.985	13.538	15.094	1.00	0.00	H
ATOM	778	1HB	ARG	172	26.359	11.208	16.882	1.00	0.00	H
ATOM	779	2HB	ARG	172	27.478	11.196	15.484	1.00	0.00	H
ATOM	780	1HG	ARG	172	25.546	11.729	13.969	1.00	0.00	H
ATOM	781	2HG	ARG	172	24.462	11.741	15.323	1.00	0.00	H
ATOM	782	1HD	ARG	172	24.949	9.410	15.774	1.00	0.00	H
ATOM	783	2HD	ARG	172	26.073	9.398	14.371	1.00	0.00	H
ATOM	784	HE	ARG	172	23.464	10.491	13.574	1.00	0.00	H
ATOM	785	1HH1	ARG	172	25.189	7.453	14.461	1.00	0.00	H
ATOM	786	2HH1	ARG	172	24.144	6.400	13.471	1.00	0.00	H
ATOM	787	1HH2	ARG	172	22.080	9.091	12.258	1.00	0.00	H
ATOM	788	2HH2	ARG	172	22.374	7.332	12.217	1.00	0.00	H
ATOM	789	N	MET	173	25.574	15.121	16.643	1.00	0.00	N
ATOM	790	CA	MET	173	24.514	15.985	17.080	1.00	0.00	C
ATOM	791	C	MET	173	23.271	15.956	16.207	1.00	0.00	C
ATOM	792	O	MET	173	22.220	16.236	16.781	1.00	0.00	O
ATOM	793	CB	MET	173	24.965	17.453	17.143	1.00	0.00	C
ATOM	794	CG	MET	173	26.131	17.692	18.105	1.00	0.00	C
ATOM	795	SD	MET	173	27.725	17.037	17.523	1.00	0.00	S
ATOM	796	CE	MET	173	27.899	18.244	16.176	1.00	0.00	C
ATOM	797	H	MET	173	26.419	15.585	16.281	1.00	0.00	H
ATOM	798	HA	MET	173	24.217	15.679	18.083	1.00	0.00	H
ATOM	799	1HB	MET	173	24.180	18.134	17.470	1.00	0.00	H
ATOM	800	2HB	MET	173	25.301	17.845	16.183	1.00	0.00	H
ATOM	801	1HG	MET	173	25.898	17.205	19.052	1.00	0.00	H
ATOM	802	2HG	MET	173	26.245	18.767	18.244	1.00	0.00	H
ATOM	803	1HE	MET	173	27.038	18.913	16.173	1.00	0.00	H
ATOM	804	2HE	MET	173	28.809	18.824	16.323	1.00	0.00	H
ATOM	805	3HE	MET	173	27.953	17.719	15.222	1.00	0.00	H
ATOM	806	N	PRO	174	23.232	15.682	14.906	1.00	0.00	N
ATOM	807	CA	PRO	174	22.027	15.893	14.140	1.00	0.00	C
ATOM	808	C	PRO	174	20.773	15.279	14.674	1.00	0.00	C
ATOM	809	O	PRO	174	19.710	15.754	14.285	1.00	0.00	O
ATOM	810	CB	PRO	174	22.314	15.362	12.737	1.00	0.00	C
ATOM	811	CG	PRO	174	23.324	14.239	12.993	1.00	0.00	C

ATOM	812	CD	PRO	174	24.105	14.737	14.215	1.00	0.00	C
ATOM	813	HA	PRO	174	21.852	16.967	14.086	1.00	0.00	H
ATOM	814	1HB	PRO	174	22.727	16.142	12.098	1.00	0.00	H
ATOM	815	2HB	PRO	174	21.404	14.991	12.263	1.00	0.00	H
ATOM	816	1HG	PRO	174	23.973	14.092	12.129	1.00	0.00	H
ATOM	817	2HG	PRO	174	22.817	13.295	13.193	1.00	0.00	H
ATOM	818	1HD	PRO	174	24.317	13.937	14.925	1.00	0.00	H
ATOM	819	2HD	PRO	174	25.000	15.292	13.936	1.00	0.00	H
ATOM	820	N	LEU	175	20.820	14.229	15.513	1.00	0.00	N
ATOM	821	CA	LEU	175	19.557	13.719	15.967	1.00	0.00	C
ATOM	822	C	LEU	175	18.856	14.813	16.709	1.00	0.00	C
ATOM	823	O	LEU	175	17.668	15.054	16.501	1.00	0.00	O
ATOM	824	CB	LEU	175	19.682	12.496	16.893	1.00	0.00	C
ATOM	825	CG	LEU	175	20.153	11.228	16.156	1.00	0.00	C
ATOM	826	CD1	LEU	175	19.103	10.760	15.135	1.00	0.00	C
ATOM	827	CD2	LEU	175	21.543	11.421	15.532	1.00	0.00	C
ATOM	828	H	LEU	175	21.713	13.813	15.813	1.00	0.00	H
ATOM	829	HA	LEU	175	18.983	13.412	15.092	1.00	0.00	H
ATOM	830	1HB	LEU	175	18.740	12.226	17.372	1.00	0.00	H
ATOM	831	2HB	LEU	175	20.393	12.646	17.704	1.00	0.00	H
ATOM	832	HG	LEU	175	20.326	10.410	16.855	1.00	0.00	H
ATOM	833	1HD1	LEU	175	18.247	11.435	15.157	1.00	0.00	H
ATOM	834	2HD1	LEU	175	19.540	10.761	14.136	1.00	0.00	H
ATOM	835	3HD1	LEU	175	18.775	9.751	15.386	1.00	0.00	H
ATOM	836	1HD2	LEU	175	21.902	12.427	15.747	1.00	0.00	H
ATOM	837	2HD2	LEU	175	22.234	10.691	15.952	1.00	0.00	H
ATOM	838	3HD2	LEU	175	21.479	11.281	14.452	1.00	0.00	H
ATOM	839	N	ILE	176	19.582	15.505	17.603	1.00	0.00	N
ATOM	840	CA	ILE	176	19.021	16.602	18.332	1.00	0.00	C
ATOM	841	C	ILE	176	18.856	17.761	17.396	1.00	0.00	C
ATOM	842	O	ILE	176	17.894	18.522	17.484	1.00	0.00	O
ATOM	843	CB	ILE	176	19.889	17.028	19.481	1.00	0.00	C
ATOM	844	CG1	ILE	176	19.109	17.948	20.433	1.00	0.00	C
ATOM	845	CG2	ILE	176	21.181	17.642	18.914	1.00	0.00	C
ATOM	846	CD1	ILE	176	19.795	18.154	21.784	1.00	0.00	C
ATOM	847	H	ILE	176	20.563	15.240	17.767	1.00	0.00	H
ATOM	848	HA	ILE	176	18.054	16.294	18.730	1.00	0.00	H
ATOM	849	HB	ILE	176	20.117	16.149	20.085	1.00	0.00	H
ATOM	850	1HG1	ILE	176	18.111	17.580	20.675	1.00	0.00	H
ATOM	851	2HG1	ILE	176	18.952	18.952	20.038	1.00	0.00	H
ATOM	852	1HG2	ILE	176	21.148	17.616	17.824	1.00	0.00	H
ATOM	853	2HG2	ILE	176	21.271	18.674	19.250	1.00	0.00	H
ATOM	854	3HG2	ILE	176	22.040	17.070	19.264	1.00	0.00	H
ATOM	855	1HD1	ILE	176	20.728	17.592	21.807	1.00	0.00	H
ATOM	856	2HD1	ILE	176	20.005	19.213	21.927	1.00	0.00	H
ATOM	857	3HD1	ILE	176	19.140	17.803	22.581	1.00	0.00	H
ATOM	858	N	GLU	177	19.806	17.900	16.455	1.00	0.00	N
ATOM	859	CA	GLU	177	19.880	19.007	15.542	1.00	0.00	C
ATOM	860	C	GLU	177	18.707	19.040	14.608	1.00	0.00	C
ATOM	861	O	GLU	177	18.246	20.115	14.227	1.00	0.00	O
ATOM	862	CB	GLU	177	21.183	18.981	14.714	1.00	0.00	C
ATOM	863	CG	GLU	177	21.468	20.288	13.969	1.00	0.00	C
ATOM	864	CD	GLU	177	22.934	20.298	13.545	1.00	0.00	C
ATOM	865	OE1	GLU	177	23.550	19.200	13.498	1.00	0.00	O
ATOM	866	OE2	GLU	177	23.457	21.411	13.266	1.00	0.00	O
ATOM	867	H	GLU	177	20.526	17.166	16.384	1.00	0.00	H
ATOM	868	HA	GLU	177	19.897	19.963	16.064	1.00	0.00	H
ATOM	869	1HB	GLU	177	21.198	18.211	13.942	1.00	0.00	H
ATOM	870	2HB	GLU	177	22.078	18.798	15.308	1.00	0.00	H
ATOM	871	1HG	GLU	177	21.262	21.122	14.639	1.00	0.00	H
ATOM	872	2HG	GLU	177	20.820	20.338	13.093	1.00	0.00	H
ATOM	873	N	LEU	178	18.171	17.867	14.229	1.00	0.00	N
ATOM	874	CA	LEU	178	17.164	17.780	13.210	1.00	0.00	C
ATOM	875	C	LEU	178	15.945	18.581	13.544	1.00	0.00	C
ATOM	876	O	LEU	178	15.455	19.334	12.706	1.00	0.00	O
ATOM	877	CB	LEU	178	16.678	16.342	12.969	1.00	0.00	C
ATOM	878	CG	LEU	178	17.748	15.383	12.413	1.00	0.00	C
ATOM	879	CD1	LEU	178	17.169	13.975	12.197	1.00	0.00	C

ATOM	880	CD2	LEU	178	18.419	15.956	11.154	1.00	0.00	C
ATOM	881	H	LEU	178	18.493	17.001	14.685	1.00	0.00	H
ATOM	882	HA	LEU	178	17.517	18.144	12.245	1.00	0.00	H
ATOM	883	1HB	LEU	178	15.861	16.375	12.247	1.00	0.00	H
ATOM	884	2HB	LEU	178	16.335	15.934	13.920	1.00	0.00	H
ATOM	885	HG	LEU	178	18.590	15.296	13.099	1.00	0.00	H
ATOM	886	1HD1	LEU	178	16.118	13.965	12.487	1.00	0.00	H
ATOM	887	2HD1	LEU	178	17.257	13.702	11.145	1.00	0.00	H
ATOM	888	3HD1	LEU	178	17.720	13.257	12.804	1.00	0.00	H
ATOM	889	1HD2	LEU	178	17.987	16.930	10.923	1.00	0.00	H
ATOM	890	2HD2	LEU	178	19.489	16.065	11.330	1.00	0.00	H
ATOM	891	3HD2	LEU	178	18.256	15.279	10.315	1.00	0.00	H
ATOM	892	N	GLY	179	15.415	18.479	14.776	1.00	0.00	N
ATOM	893	CA	GLY	179	14.154	19.139	14.949	1.00	0.00	C
ATOM	894	C	GLY	179	14.199	20.110	16.075	1.00	0.00	C
ATOM	895	O	GLY	179	13.695	21.225	15.954	1.00	0.00	O
ATOM	896	H	GLY	179	15.880	17.965	15.538	1.00	0.00	H
ATOM	897	1HA	GLY	179	13.357	18.426	15.163	1.00	0.00	H
ATOM	898	2HA	GLY	179	13.866	19.690	14.053	1.00	0.00	H
ATOM	899	N	PRO	180	14.773	19.733	17.174	1.00	0.00	N
ATOM	900	CA	PRO	180	14.743	20.627	18.289	1.00	0.00	C
ATOM	901	C	PRO	180	15.493	21.892	18.046	1.00	0.00	C
ATOM	902	O	PRO	180	15.199	22.883	18.711	1.00	0.00	O
ATOM	903	CB	PRO	180	15.172	19.808	19.511	1.00	0.00	C
ATOM	904	CG	PRO	180	15.490	18.403	18.955	1.00	0.00	C
ATOM	905	CD	PRO	180	14.745	18.351	17.613	1.00	0.00	C
ATOM	906	HA	PRO	180	13.734	20.933	18.565	1.00	0.00	H
ATOM	907	1HB	PRO	180	14.310	19.829	20.178	1.00	0.00	H
ATOM	908	2HB	PRO	180	16.044	20.329	19.905	1.00	0.00	H
ATOM	909	1HG	PRO	180	15.098	17.721	19.709	1.00	0.00	H
ATOM	910	2HG	PRO	180	16.576	18.390	18.863	1.00	0.00	H
ATOM	911	1HD	PRO	180	15.243	17.700	16.894	1.00	0.00	H
ATOM	912	2HD	PRO	180	13.721	17.995	17.728	1.00	0.00	H
ATOM	913	N	LEU	181	16.467	21.893	17.121	1.00	0.00	N
ATOM	914	CA	LEU	181	17.165	23.111	16.833	1.00	0.00	C
ATOM	915	C	LEU	181	16.199	24.075	16.231	1.00	0.00	C
ATOM	916	O	LEU	181	16.226	25.266	16.537	1.00	0.00	O
ATOM	917	CB	LEU	181	18.337	22.920	15.859	1.00	0.00	C
ATOM	918	CG	LEU	181	19.575	22.321	16.546	1.00	0.00	C
ATOM	919	CD1	LEU	181	20.341	23.397	17.335	1.00	0.00	C
ATOM	920	CD2	LEU	181	19.181	21.138	17.444	1.00	0.00	C
ATOM	921	H	LEU	181	16.710	21.025	16.622	1.00	0.00	H
ATOM	922	HA	LEU	181	17.567	23.504	17.766	1.00	0.00	H
ATOM	923	1HB	LEU	181	18.657	23.859	15.408	1.00	0.00	H
ATOM	924	2HB	LEU	181	18.086	22.251	15.035	1.00	0.00	H
ATOM	925	HG	LEU	181	20.258	21.891	15.813	1.00	0.00	H
ATOM	926	1HD1	LEU	181	19.832	24.355	17.231	1.00	0.00	H
ATOM	927	2HD1	LEU	181	20.379	23.118	18.388	1.00	0.00	H
ATOM	928	3HD1	LEU	181	21.355	23.481	16.945	1.00	0.00	H
ATOM	929	1HD2	LEU	181	18.102	20.986	17.393	1.00	0.00	H
ATOM	930	2HD2	LEU	181	19.690	20.236	17.103	1.00	0.00	H
ATOM	931	3HD2	LEU	181	19.469	21.350	18.473	1.00	0.00	H
ATOM	932	N	ARG	182	15.300	23.579	15.363	1.00	0.00	N
ATOM	933	CA	ARG	182	14.348	24.458	14.756	1.00	0.00	C
ATOM	934	C	ARG	182	13.540	25.045	15.861	1.00	0.00	C
ATOM	935	O	ARG	182	13.199	26.227	15.836	1.00	0.00	O
ATOM	936	CB	ARG	182	13.385	23.745	13.789	1.00	0.00	C
ATOM	937	CG	ARG	182	12.366	24.688	13.144	1.00	0.00	C
ATOM	938	CD	ARG	182	11.503	24.028	12.065	1.00	0.00	C
ATOM	939	NE	ARG	182	12.360	23.836	10.860	1.00	0.00	N
ATOM	940	CZ	ARG	182	11.960	23.000	9.857	1.00	0.00	C
ATOM	941	NH1	ARG	182	10.785	22.314	9.967	1.00	0.00	N
ATOM	942	NH2	ARG	182	12.736	22.850	8.745	1.00	0.00	N
ATOM	943	H	ARG	182	15.296	22.574	15.136	1.00	0.00	H
ATOM	944	HA	ARG	182	14.918	25.216	14.218	1.00	0.00	H
ATOM	945	1HB	ARG	182	12.793	22.963	14.267	1.00	0.00	H
ATOM	946	2HB	ARG	182	13.892	23.255	12.957	1.00	0.00	H
ATOM	947	1HG	ARG	182	12.906	25.512	12.679	1.00	0.00	H

ATOM	948	2HG	ARG	182	11.699	25.058	13.922	1.00	0.00	H
ATOM	949	1HD	ARG	182	10.669	24.698	11.856	1.00	0.00	H
ATOM	950	2HD	ARG	182	11.155	23.073	12.461	1.00	0.00	H
ATOM	951	HE	ARG	182	13.257	24.335	10.783	1.00	0.00	H
ATOM	952	1HH1	ARG	182	10.199	22.426	10.806	1.00	0.00	H
ATOM	953	2HH1	ARG	182	10.483	21.683	9.210	1.00	0.00	H
ATOM	954	1HH2	ARG	182	13.622	23.367	8.662	1.00	0.00	H
ATOM	955	2HH2	ARG	182	12.435	22.219	7.988	1.00	0.00	H
ATOM	956	N	SER	183	13.226	24.222	16.878	1.00	0.00	N
ATOM	957	CA	SER	183	12.450	24.713	17.975	1.00	0.00	C
ATOM	958	C	SER	183	13.184	25.875	18.559	1.00	0.00	C
ATOM	959	O	SER	183	14.397	25.840	18.757	1.00	0.00	O
ATOM	960	CB	SER	183	12.239	23.679	19.093	1.00	0.00	C
ATOM	961	OG	SER	183	11.487	22.579	18.603	1.00	0.00	O
ATOM	962	H	SER	183	13.543	23.242	16.866	1.00	0.00	H
ATOM	963	HA	SER	183	11.479	25.013	17.580	1.00	0.00	H
ATOM	964	1HB	SER	183	11.699	24.132	19.924	1.00	0.00	H
ATOM	965	2HB	SER	183	13.201	23.316	19.452	1.00	0.00	H
ATOM	966	HG	SER	183	10.552	22.902	18.314	1.00	0.00	H
ATOM	967	N	PHE	184	12.430	26.948	18.842	1.00	0.00	N
ATOM	968	CA	PHE	184	12.934	28.161	19.411	1.00	0.00	C
ATOM	969	C	PHE	184	13.337	27.865	20.818	1.00	0.00	C
ATOM	970	O	PHE	184	14.090	28.618	21.433	1.00	0.00	O
ATOM	971	CB	PHE	184	11.890	29.294	19.429	1.00	0.00	C
ATOM	972	CG	PHE	184	10.758	28.871	20.300	1.00	0.00	C
ATOM	973	CD1	PHE	184	10.795	29.107	21.654	1.00	0.00	C
ATOM	974	CD2	PHE	184	9.659	28.240	19.763	1.00	0.00	C
ATOM	975	CE1	PHE	184	9.754	28.719	22.463	1.00	0.00	C
ATOM	976	CE2	PHE	184	8.614	27.849	20.567	1.00	0.00	C
ATOM	977	CZ	PHE	184	8.660	28.088	21.920	1.00	0.00	C
ATOM	978	H	PHE	184	11.422	26.895	18.636	1.00	0.00	H
ATOM	979	HA	PHE	184	13.788	28.475	18.811	1.00	0.00	H
ATOM	980	1HB	PHE	184	11.548	29.459	18.407	1.00	0.00	H
ATOM	981	2HB	PHE	184	12.366	30.190	19.825	1.00	0.00	H
ATOM	982	HD1	PHE	184	11.659	29.607	22.090	1.00	0.00	H
ATOM	983	HD2	PHE	184	9.616	28.048	18.690	1.00	0.00	H
ATOM	984	HE1	PHE	184	9.795	28.911	23.535	1.00	0.00	H
ATOM	985	HE2	PHE	184	7.748	27.349	20.131	1.00	0.00	H
ATOM	986	HZ	PHE	184	7.833	27.778	22.559	1.00	0.00	H
ATOM	987	N	LYS	185	12.840	26.733	21.350	1.00	0.00	N
ATOM	988	CA	LYS	185	12.976	26.395	22.738	1.00	0.00	C
ATOM	989	C	LYS	185	14.390	26.554	23.216	1.00	0.00	C
ATOM	990	O	LYS	185	14.618	27.336	24.138	1.00	0.00	O
ATOM	991	CB	LYS	185	12.595	24.932	23.006	1.00	0.00	C
ATOM	992	CG	LYS	185	11.125	24.603	22.741	1.00	0.00	C
ATOM	993	CD	LYS	185	10.152	25.346	23.658	1.00	0.00	C
ATOM	994	CE	LYS	185	8.684	25.009	23.392	1.00	0.00	C
ATOM	995	NZ	LYS	185	7.824	25.699	24.378	1.00	0.00	N
ATOM	996	H	LYS	185	12.338	26.078	20.732	1.00	0.00	H
ATOM	997	HA	LYS	185	12.352	27.025	23.372	1.00	0.00	H
ATOM	998	1HB	LYS	185	12.798	24.712	24.054	1.00	0.00	H
ATOM	999	2HB	LYS	185	13.197	24.297	22.356	1.00	0.00	H
ATOM	1000	1HG	LYS	185	10.880	23.548	22.870	1.00	0.00	H
ATOM	1001	2HG	LYS	185	10.796	24.844	21.730	1.00	0.00	H
ATOM	1002	1HD	LYS	185	10.214	26.430	23.571	1.00	0.00	H
ATOM	1003	2HD	LYS	185	10.304	25.135	24.716	1.00	0.00	H
ATOM	1004	1HE	LYS	185	8.530	23.933	23.475	1.00	0.00	H
ATOM	1005	2HE	LYS	185	8.406	25.331	22.388	1.00	0.00	H
ATOM	1006	1HZ	LYS	185	8.411	26.250	25.020	1.00	0.00	H
ATOM	1007	2HZ	LYS	185	7.171	26.326	23.886	1.00	0.00	H
ATOM	1008	3HZ	LYS	185	7.289	25.001	24.915	1.00	0.00	H
ATOM	1009	N	VAL	186	15.396	25.856	22.641	1.00	0.00	N
ATOM	1010	CA	VAL	186	16.684	26.128	23.228	1.00	0.00	C
ATOM	1011	C	VAL	186	17.800	25.513	22.438	1.00	0.00	C
ATOM	1012	O	VAL	186	17.576	24.723	21.522	1.00	0.00	O
ATOM	1013	CB	VAL	186	16.866	25.589	24.611	1.00	0.00	C
ATOM	1014	CG1	VAL	186	17.191	24.091	24.500	1.00	0.00	C
ATOM	1015	CG2	VAL	186	17.939	26.411	25.342	1.00	0.00	C

ATOM	1016	H	VAL	186	15.255	25.196	21.862	1.00	0.00	H
ATOM	1017	HA	VAL	186	16.887	27.197	23.285	1.00	0.00	H
ATOM	1018	HB	VAL	186	15.937	25.744	25.159	1.00	0.00	H
ATOM	1019	1HG1	VAL	186	17.207	23.799	23.450	1.00	0.00	H
ATOM	1020	2HG1	VAL	186	18.166	23.896	24.945	1.00	0.00	H
ATOM	1021	3HG1	VAL	186	16.430	23.513	25.025	1.00	0.00	H
ATOM	1022	1HG2	VAL	186	18.313	27.191	24.679	1.00	0.00	H
ATOM	1023	2HG2	VAL	186	17.504	26.867	26.231	1.00	0.00	H
ATOM	1024	3HG2	VAL	186	18.761	25.758	25.633	1.00	0.00	H
ATOM	1025	N	PHE	187	19.048	25.904	22.793	1.00	0.00	N
ATOM	1026	CA	PHE	187	20.262	25.391	22.216	1.00	0.00	C
ATOM	1027	C	PHE	187	21.286	26.460	22.477	1.00	0.00	C
ATOM	1028	O	PHE	187	21.009	27.384	23.239	1.00	0.00	O
ATOM	1029	CB	PHE	187	20.152	25.175	20.689	1.00	0.00	C
ATOM	1030	CG	PHE	187	21.285	24.332	20.203	1.00	0.00	C
ATOM	1031	CD1	PHE	187	21.291	22.977	20.443	1.00	0.00	C
ATOM	1032	CD2	PHE	187	22.322	24.877	19.478	1.00	0.00	C
ATOM	1033	CE1	PHE	187	22.324	22.185	19.996	1.00	0.00	C
ATOM	1034	CE2	PHE	187	23.357	24.091	19.029	1.00	0.00	C
ATOM	1035	CZ	PHE	187	23.362	22.742	19.291	1.00	0.00	C
ATOM	1036	H	PHE	187	19.133	26.619	23.528	1.00	0.00	H
ATOM	1037	HA	PHE	187	20.448	24.460	22.752	1.00	0.00	H
ATOM	1038	1HB	PHE	187	20.181	26.132	20.169	1.00	0.00	H
ATOM	1039	2HB	PHE	187	19.215	24.674	20.445	1.00	0.00	H
ATOM	1040	HD1	PHE	187	20.466	22.524	20.994	1.00	0.00	H
ATOM	1041	HD2	PHE	187	22.322	25.944	19.257	1.00	0.00	H
ATOM	1042	HE1	PHE	187	22.318	21.114	20.201	1.00	0.00	H
ATOM	1043	HE2	PHE	187	24.174	24.538	18.464	1.00	0.00	H
ATOM	1044	HZ	PHE	187	24.184	22.118	18.941	1.00	0.00	H
ATOM	1045	N	LYS	188	22.500	26.319	21.890	1.00	0.00	N
ATOM	1046	CA	LYS	188	23.583	27.276	21.893	1.00	0.00	C
ATOM	1047	C	LYS	188	24.870	26.565	22.163	1.00	0.00	C
ATOM	1048	O	LYS	188	24.885	25.410	22.586	1.00	0.00	O
ATOM	1049	CB	LYS	188	23.496	28.450	22.890	1.00	0.00	C
ATOM	1050	CG	LYS	188	22.508	29.554	22.501	1.00	0.00	C
ATOM	1051	CD	LYS	188	22.239	30.545	23.634	1.00	0.00	C
ATOM	1052	CE	LYS	188	21.535	29.916	24.838	1.00	0.00	C
ATOM	1053	NZ	LYS	188	21.318	30.934	25.890	1.00	0.00	N
ATOM	1054	H	LYS	188	22.668	25.435	21.388	1.00	0.00	H
ATOM	1055	HA	LYS	188	23.632	27.767	20.921	1.00	0.00	H
ATOM	1056	1HB	LYS	188	24.483	28.906	22.964	1.00	0.00	H
ATOM	1057	2HB	LYS	188	23.179	28.053	23.854	1.00	0.00	H
ATOM	1058	1HG	LYS	188	21.530	29.169	22.209	1.00	0.00	H
ATOM	1059	2HG	LYS	188	22.849	30.156	21.659	1.00	0.00	H
ATOM	1060	1HD	LYS	188	21.606	31.381	23.337	1.00	0.00	H
ATOM	1061	2HD	LYS	188	23.144	30.999	24.036	1.00	0.00	H
ATOM	1062	1HE	LYS	188	22.142	29.110	25.249	1.00	0.00	H
ATOM	1063	2HE	LYS	188	20.569	29.509	24.537	1.00	0.00	H
ATOM	1064	1HZ	LYS	188	21.691	31.840	25.573	1.00	0.00	H
ATOM	1065	2HZ	LYS	188	20.309	31.025	26.077	1.00	0.00	H
ATOM	1066	3HZ	LYS	188	21.802	30.646	26.752	1.00	0.00	H
ATOM	1067	N	ILE	189	25.996	27.260	21.897	1.00	0.00	N
ATOM	1068	CA	ILE	189	27.304	26.713	22.113	1.00	0.00	C
ATOM	1069	C	ILE	189	27.526	26.621	23.583	1.00	0.00	C
ATOM	1070	O	ILE	189	28.132	25.670	24.075	1.00	0.00	O
ATOM	1071	CB	ILE	189	28.414	27.572	21.575	1.00	0.00	C
ATOM	1072	CG1	ILE	189	28.312	27.716	20.048	1.00	0.00	C
ATOM	1073	CG2	ILE	189	29.747	26.968	22.052	1.00	0.00	C
ATOM	1074	CD1	ILE	189	29.257	28.773	19.478	1.00	0.00	C
ATOM	1075	H	ILE	189	25.912	28.217	21.525	1.00	0.00	H
ATOM	1076	HA	ILE	189	27.335	25.726	21.651	1.00	0.00	H
ATOM	1077	HB	ILE	189	28.274	28.578	21.968	1.00	0.00	H
ATOM	1078	1HG1	ILE	189	27.316	28.002	19.708	1.00	0.00	H
ATOM	1079	2HG1	ILE	189	28.547	26.796	19.512	1.00	0.00	H
ATOM	1080	1HG2	ILE	189	29.549	26.080	22.652	1.00	0.00	H
ATOM	1081	2HG2	ILE	189	30.352	26.694	21.187	1.00	0.00	H
ATOM	1082	3HG2	ILE	189	30.284	27.701	22.653	1.00	0.00	H
ATOM	1083	1HD1	ILE	189	29.828	29.224	20.288	1.00	0.00	H

ATOM	1084	2HD1	ILE	189	29.940	28.305	18.768	1.00	0.00	H
ATOM	1085	3HD1	ILE	189	28.677	29.543	18.969	1.00	0.00	H
ATOM	1086	N	LYS	190	27.035	27.629	24.324	1.00	0.00	N
ATOM	1087	CA	LYS	190	27.213	27.664	25.745	1.00	0.00	C
ATOM	1088	C	LYS	190	26.543	26.467	26.343	1.00	0.00	C
ATOM	1089	O	LYS	190	27.070	25.870	27.280	1.00	0.00	O
ATOM	1090	CB	LYS	190	26.635	28.933	26.394	1.00	0.00	C
ATOM	1091	CG	LYS	190	26.988	29.068	27.877	1.00	0.00	C
ATOM	1092	CD	LYS	190	26.785	30.479	28.432	1.00	0.00	C
ATOM	1093	CE	LYS	190	27.971	31.413	28.171	1.00	0.00	C
ATOM	1094	NZ	LYS	190	28.057	31.738	26.730	1.00	0.00	N
ATOM	1095	H	LYS	190	26.520	28.391	23.860	1.00	0.00	H
ATOM	1096	HA	LYS	190	28.280	27.646	25.964	1.00	0.00	H
ATOM	1097	1HB	LYS	190	25.547	28.982	26.349	1.00	0.00	H
ATOM	1098	2HB	LYS	190	26.986	29.853	25.927	1.00	0.00	H
ATOM	1099	1HG	LYS	190	28.025	28.823	28.104	1.00	0.00	H
ATOM	1100	2HG	LYS	190	26.398	28.423	28.528	1.00	0.00	H
ATOM	1101	1HD	LYS	190	26.633	30.502	29.511	1.00	0.00	H
ATOM	1102	2HD	LYS	190	25.919	30.990	28.010	1.00	0.00	H
ATOM	1103	1HE	LYS	190	28.900	30.934	28.478	1.00	0.00	H
ATOM	1104	2HE	LYS	190	27.850	32.339	28.732	1.00	0.00	H
ATOM	1105	1HZ	LYS	190	27.297	31.261	26.224	1.00	0.00	H
ATOM	1106	2HZ	LYS	190	27.968	32.756	26.601	1.00	0.00	H
ATOM	1107	3HZ	LYS	190	28.965	31.423	26.360	1.00	0.00	H
ATOM	1108	N	PRO	191	25.406	26.078	25.838	1.00	0.00	N
ATOM	1109	CA	PRO	191	24.785	24.909	26.381	1.00	0.00	C
ATOM	1110	C	PRO	191	25.649	23.721	26.128	1.00	0.00	C
ATOM	1111	O	PRO	191	25.410	22.675	26.728	1.00	0.00	O
ATOM	1112	CB	PRO	191	23.391	24.869	25.766	1.00	0.00	C
ATOM	1113	CG	PRO	191	23.050	26.360	25.589	1.00	0.00	C
ATOM	1114	CD	PRO	191	24.413	27.047	25.405	1.00	0.00	C
ATOM	1115	HA	PRO	191	24.647	25.033	27.455	1.00	0.00	H
ATOM	1116	1HB	PRO	191	22.684	24.364	26.425	1.00	0.00	H
ATOM	1117	2HB	PRO	191	23.396	24.336	24.815	1.00	0.00	H
ATOM	1118	1HG	PRO	191	22.537	26.633	26.511	1.00	0.00	H
ATOM	1119	2HG	PRO	191	22.415	26.391	24.703	1.00	0.00	H
ATOM	1120	1HD	PRO	191	24.642	27.260	24.361	1.00	0.00	H
ATOM	1121	2HD	PRO	191	24.541	27.913	26.053	1.00	0.00	H
ATOM	1122	N	GLU	192	26.651	23.854	25.242	1.00	0.00	N
ATOM	1123	CA	GLU	192	27.569	22.774	25.046	1.00	0.00	C
ATOM	1124	C	GLU	192	28.727	23.091	25.928	1.00	0.00	C
ATOM	1125	O	GLU	192	29.185	24.232	25.968	1.00	0.00	O
ATOM	1126	CB	GLU	192	28.119	22.653	23.615	1.00	0.00	C
ATOM	1127	CG	GLU	192	27.073	22.223	22.586	1.00	0.00	C
ATOM	1128	CD	GLU	192	27.796	21.960	21.272	1.00	0.00	C
ATOM	1129	OE1	GLU	192	28.458	22.898	20.753	1.00	0.00	O
ATOM	1130	OE2	GLU	192	27.705	20.807	20.772	1.00	0.00	O
ATOM	1131	H	GLU	192	26.757	24.728	24.707	1.00	0.00	H
ATOM	1132	HA	GLU	192	27.020	21.881	25.348	1.00	0.00	H
ATOM	1133	1HB	GLU	192	28.924	21.926	23.513	1.00	0.00	H
ATOM	1134	2HB	GLU	192	28.530	23.582	23.221	1.00	0.00	H
ATOM	1135	1HG	GLU	192	26.354	23.036	22.483	1.00	0.00	H
ATOM	1136	2HG	GLU	192	26.593	21.318	22.958	1.00	0.00	H
ATOM	1137	N	LYS	193	29.226	22.090	26.676	1.00	0.00	N
ATOM	1138	CA	LYS	193	30.300	22.366	27.583	1.00	0.00	C
ATOM	1139	C	LYS	193	31.517	22.676	26.770	1.00	0.00	C
ATOM	1140	O	LYS	193	32.251	21.775	26.365	1.00	0.00	O
ATOM	1141	CB	LYS	193	30.616	21.189	28.517	1.00	0.00	C
ATOM	1142	CG	LYS	193	29.422	20.775	29.380	1.00	0.00	C
ATOM	1143	CD	LYS	193	28.864	21.913	30.235	1.00	0.00	C
ATOM	1144	CE	LYS	193	28.068	22.942	29.429	1.00	0.00	C
ATOM	1145	NZ	LYS	193	27.558	24.004	30.323	1.00	0.00	N
ATOM	1146	H	LYS	193	28.840	21.137	26.597	1.00	0.00	H
ATOM	1147	HA	LYS	193	30.008	23.220	28.194	1.00	0.00	H
ATOM	1148	1HB	LYS	193	31.425	21.405	29.214	1.00	0.00	H
ATOM	1149	2HB	LYS	193	30.919	20.290	27.980	1.00	0.00	H
ATOM	1150	1HG	LYS	193	29.651	19.975	30.084	1.00	0.00	H
ATOM	1151	2HG	LYS	193	28.573	20.410	28.801	1.00	0.00	H

ATOM	1152	1HD	LYS	193	29.636	22.484	30.750	1.00	0.00	H
ATOM	1153	2HD	LYS	193	28.186	21.572	31.017	1.00	0.00	H
ATOM	1154	1HE	LYS	193	27.222	22.460	28.937	1.00	0.00	H
ATOM	1155	2HE	LYS	193	28.704	23.396	28.669	1.00	0.00	H
ATOM	1156	1HZ	LYS	193	27.854	23.811	31.290	1.00	0.00	H
ATOM	1157	2HZ	LYS	193	27.934	24.915	30.024	1.00	0.00	H
ATOM	1158	3HZ	LYS	193	26.529	24.026	30.277	1.00	0.00	H
ATOM	1159	N	ARG	194	31.741	23.979	26.494	1.00	0.00	N
ATOM	1160	CA	ARG	194	32.867	24.397	25.713	1.00	0.00	C
ATOM	1161	C	ARG	194	34.107	24.240	26.526	1.00	0.00	C
ATOM	1162	O	ARG	194	35.099	23.690	26.051	1.00	0.00	O
ATOM	1163	CB	ARG	194	32.793	25.871	25.273	1.00	0.00	C
ATOM	1164	CG	ARG	194	32.765	26.874	26.429	1.00	0.00	C
ATOM	1165	CD	ARG	194	32.708	28.332	25.962	1.00	0.00	C
ATOM	1166	NE	ARG	194	32.685	29.199	27.173	1.00	0.00	N
ATOM	1167	CZ	ARG	194	32.910	30.540	27.058	1.00	0.00	C
ATOM	1168	NH1	ARG	194	33.179	31.085	25.836	1.00	0.00	N
ATOM	1169	NH2	ARG	194	32.863	31.338	28.165	1.00	0.00	N
ATOM	1170	H	ARG	194	31.086	24.688	26.853	1.00	0.00	H
ATOM	1171	HA	ARG	194	32.928	23.777	24.818	1.00	0.00	H
ATOM	1172	1HB	ARG	194	31.880	26.009	24.693	1.00	0.00	H
ATOM	1173	2HB	ARG	194	33.671	26.091	24.665	1.00	0.00	H
ATOM	1174	1HG	ARG	194	33.640	26.809	27.075	1.00	0.00	H
ATOM	1175	2HG	ARG	194	31.906	26.745	27.088	1.00	0.00	H
ATOM	1176	1HD	ARG	194	31.799	28.459	25.372	1.00	0.00	H
ATOM	1177	2HD	ARG	194	33.595	28.525	25.359	1.00	0.00	H
ATOM	1178	HE	ARG	194	32.499	28.785	28.098	1.00	0.00	H
ATOM	1179	1HH1	ARG	194	33.212	30.484	25.000	1.00	0.00	H
ATOM	1180	2HH1	ARG	194	33.348	32.097	25.749	1.00	0.00	H
ATOM	1181	1HH2	ARG	194	32.657	30.927	29.087	1.00	0.00	H
ATOM	1182	2HH2	ARG	194	33.033	32.350	28.077	1.00	0.00	H
ATOM	1183	N	TRP	195	34.072	24.705	27.790	1.00	0.00	N
ATOM	1184	CA	TRP	195	35.243	24.637	28.613	1.00	0.00	C
ATOM	1185	C	TRP	195	35.661	23.212	28.692	1.00	0.00	C
ATOM	1186	O	TRP	195	36.778	22.858	28.320	1.00	0.00	O
ATOM	1187	CB	TRP	195	34.987	25.126	30.050	1.00	0.00	C
ATOM	1188	CG	TRP	195	36.189	25.050	30.963	1.00	0.00	C
ATOM	1189	CD1	TRP	195	37.206	25.941	31.148	1.00	0.00	C
ATOM	1190	CD2	TRP	195	36.447	23.951	31.849	1.00	0.00	C
ATOM	1191	NE1	TRP	195	38.082	25.461	32.093	1.00	0.00	N
ATOM	1192	CE2	TRP	195	37.626	24.236	32.535	1.00	0.00	C
ATOM	1193	CE3	TRP	195	35.753	22.796	32.075	1.00	0.00	C
ATOM	1194	CZ2	TRP	195	38.133	23.369	33.460	1.00	0.00	C
ATOM	1195	CZ3	TRP	195	36.266	21.921	33.007	1.00	0.00	C
ATOM	1196	CH2	TRP	195	37.433	22.203	33.686	1.00	0.00	C
ATOM	1197	H	TRP	195	33.202	25.109	28.165	1.00	0.00	H
ATOM	1198	HA	TRP	195	36.015	25.246	28.144	1.00	0.00	H
ATOM	1199	1HB	TRP	195	34.202	24.507	30.486	1.00	0.00	H
ATOM	1200	2HB	TRP	195	34.673	26.169	30.004	1.00	0.00	H
ATOM	1201	HD1	TRP	195	37.308	26.891	30.624	1.00	0.00	H
ATOM	1202	HE1	TRP	195	38.936	25.936	32.416	1.00	0.00	H
ATOM	1203	HE3	TRP	195	34.829	22.575	31.539	1.00	0.00	H
ATOM	1204	HZ2	TRP	195	39.054	23.590	33.998	1.00	0.00	H
ATOM	1205	HZ3	TRP	195	35.740	20.988	33.211	1.00	0.00	H
ATOM	1206	HH2	TRP	195	37.810	21.488	34.417	1.00	0.00	H
ATOM	1207	N	GLN	196	34.753	22.348	29.172	1.00	0.00	N
ATOM	1208	CA	GLN	196	35.083	20.963	29.256	1.00	0.00	C
ATOM	1209	C	GLN	196	34.251	20.260	28.238	1.00	0.00	C
ATOM	1210	O	GLN	196	33.074	19.982	28.453	1.00	0.00	O
ATOM	1211	CB	GLN	196	34.819	20.372	30.657	1.00	0.00	C
ATOM	1212	CG	GLN	196	33.366	20.482	31.127	1.00	0.00	C
ATOM	1213	CD	GLN	196	33.276	19.909	32.534	1.00	0.00	C
ATOM	1214	OE1	GLN	196	33.699	18.784	32.794	1.00	0.00	O
ATOM	1215	NE2	GLN	196	32.713	20.713	33.475	1.00	0.00	N
ATOM	1216	H	GLN	196	33.827	22.681	29.476	1.00	0.00	H
ATOM	1217	HA	GLN	196	36.148	20.879	29.041	1.00	0.00	H
ATOM	1218	1HB	GLN	196	35.439	20.906	31.375	1.00	0.00	H
ATOM	1219	2HB	GLN	196	35.079	19.313	30.636	1.00	0.00	H

ATOM	1220	1HG	GLN	196	32.741	19.912	30.438	1.00	0.00	H
ATOM	1221	2HG	GLN	196	33.084	21.535	31.121	1.00	0.00	H
ATOM	1222	1HE2	GLN	196	32.628	20.385	34.448	1.00	0.00	H
ATOM	1223	2HE2	GLN	196	32.371	21.649	33.214	1.00	0.00	H
ATOM	1224	N	ASP	197	34.851	19.958	27.074	1.00	0.00	N
ATOM	1225	CA	ASP	197	34.088	19.298	26.062	1.00	0.00	C
ATOM	1226	C	ASP	197	33.661	17.997	26.650	1.00	0.00	C
ATOM	1227	O	ASP	197	32.490	17.632	26.567	1.00	0.00	O
ATOM	1228	CB	ASP	197	34.906	19.015	24.791	1.00	0.00	C
ATOM	1229	CG	ASP	197	35.203	20.352	24.123	1.00	0.00	C
ATOM	1230	OD1	ASP	197	34.612	21.375	24.562	1.00	0.00	O
ATOM	1231	OD2	ASP	197	36.027	20.370	23.170	1.00	0.00	O
ATOM	1232	H	ASP	197	35.840	20.197	26.914	1.00	0.00	H
ATOM	1233	HA	ASP	197	33.246	19.955	25.841	1.00	0.00	H
ATOM	1234	1HB	ASP	197	34.303	18.377	24.143	1.00	0.00	H
ATOM	1235	2HB	ASP	197	35.825	18.513	25.092	1.00	0.00	H
ATOM	1236	N	ILE	198	34.631	17.292	27.269	1.00	0.00	N
ATOM	1237	CA	ILE	198	34.499	16.047	27.977	1.00	0.00	C
ATOM	1238	C	ILE	198	35.358	15.067	27.250	1.00	0.00	C
ATOM	1239	O	ILE	198	36.124	15.447	26.367	1.00	0.00	O
ATOM	1240	CB	ILE	198	33.112	15.470	28.097	1.00	0.00	C
ATOM	1241	CG1	ILE	198	33.053	14.434	29.233	1.00	0.00	C
ATOM	1242	CG2	ILE	198	32.712	14.897	26.728	1.00	0.00	C
ATOM	1243	CD1	ILE	198	33.296	15.040	30.609	1.00	0.00	C
ATOM	1244	H	ILE	198	35.578	17.693	27.229	1.00	0.00	H
ATOM	1245	HA	ILE	198	34.847	16.239	28.991	1.00	0.00	H
ATOM	1246	HB	ILE	198	32.435	16.271	28.393	1.00	0.00	H
ATOM	1247	1HG1	ILE	198	33.793	13.640	29.128	1.00	0.00	H
ATOM	1248	2HG1	ILE	198	32.089	13.928	29.302	1.00	0.00	H
ATOM	1249	1HG2	ILE	198	33.524	15.049	26.018	1.00	0.00	H
ATOM	1250	2HG2	ILE	198	32.510	13.830	26.824	1.00	0.00	H
ATOM	1251	3HG2	ILE	198	31.816	15.404	26.368	1.00	0.00	H
ATOM	1252	1HD1	ILE	198	33.467	16.111	30.509	1.00	0.00	H
ATOM	1253	2HD1	ILE	198	32.424	14.868	31.241	1.00	0.00	H
ATOM	1254	3HD1	ILE	198	34.170	14.573	31.062	1.00	0.00	H
ATOM	1255	N	SER	199	35.246	13.772	27.596	1.00	0.00	N
ATOM	1256	CA	SER	199	36.063	12.779	26.971	1.00	0.00	C
ATOM	1257	C	SER	199	35.305	11.490	26.984	1.00	0.00	C
ATOM	1258	O	SER	199	34.076	11.470	26.954	1.00	0.00	O
ATOM	1259	CB	SER	199	37.403	12.539	27.688	1.00	0.00	C
ATOM	1260	OG	SER	199	38.210	13.704	27.614	1.00	0.00	O
ATOM	1261	H	SER	199	34.565	13.493	28.317	1.00	0.00	H
ATOM	1262	HA	SER	199	36.263	13.106	25.950	1.00	0.00	H
ATOM	1263	1HB	SER	199	37.934	11.711	27.219	1.00	0.00	H
ATOM	1264	2HB	SER	199	37.227	12.297	28.736	1.00	0.00	H
ATOM	1265	HG	SER	199	39.202	13.440	27.692	1.00	0.00	H
ATOM	1266	N	MET	200	36.051	10.370	27.007	1.00	0.00	N
ATOM	1267	CA	MET	200	35.486	9.053	26.947	1.00	0.00	C
ATOM	1268	C	MET	200	34.786	8.725	28.228	1.00	0.00	C
ATOM	1269	O	MET	200	34.360	9.603	28.976	1.00	0.00	O
ATOM	1270	CB	MET	200	36.541	7.967	26.686	1.00	0.00	C
ATOM	1271	CG	MET	200	37.206	8.112	25.316	1.00	0.00	C
ATOM	1272	SD	MET	200	38.530	6.916	24.972	1.00	0.00	S
ATOM	1273	CE	MET	200	38.888	7.568	23.315	1.00	0.00	C
ATOM	1274	H	MET	200	37.074	10.462	27.070	1.00	0.00	H
ATOM	1275	HA	MET	200	34.765	8.984	26.132	1.00	0.00	H
ATOM	1276	1HB	MET	200	36.122	6.961	26.716	1.00	0.00	H
ATOM	1277	2HB	MET	200	37.347	7.982	27.419	1.00	0.00	H
ATOM	1278	1HG	MET	200	37.643	9.108	25.255	1.00	0.00	H
ATOM	1279	2HG	MET	200	36.440	7.978	24.552	1.00	0.00	H
ATOM	1280	1HE	MET	200	38.224	8.406	23.102	1.00	0.00	H
ATOM	1281	2HE	MET	200	39.923	7.904	23.272	1.00	0.00	H
ATOM	1282	3HE	MET	200	38.730	6.784	22.573	1.00	0.00	H
ATOM	1283	N	MET	201	34.643	7.410	28.486	1.00	0.00	N
ATOM	1284	CA	MET	201	33.949	6.882	29.621	1.00	0.00	C
ATOM	1285	C	MET	201	34.632	7.330	30.868	1.00	0.00	C
ATOM	1286	O	MET	201	33.966	7.659	31.846	1.00	0.00	O
ATOM	1287	CB	MET	201	33.891	5.344	29.590	1.00	0.00	C

```
ATOM   1288  CG  MET   201      35.265   4.683  29.484  1.00  0.00           C
ATOM   1289  SD  MET   201      35.204   2.915  29.066  1.00  0.00           S
ATOM   1290  CE  MET   201      34.620   3.186  27.367  1.00  0.00           C
ATOM   1291  H   MET   201      35.060   6.741  27.823  1.00  0.00           H
ATOM   1292  HA  MET   201      32.921   7.244  29.615  1.00  0.00           H
ATOM   1293 1HB  MET   201      33.319   4.946  28.751  1.00  0.00           H
ATOM   1294 2HB  MET   201      33.433   4.907  30.477  1.00  0.00           H
ATOM   1295 1HG  MET   201      35.768   4.780  30.445  1.00  0.00           H
ATOM   1296 2HG  MET   201      35.831   5.190  28.702  1.00  0.00           H
ATOM   1297 1HE  MET   201      34.510   4.255  27.186  1.00  0.00           H
ATOM   1298 2HE  MET   201      35.341   2.770  26.663  1.00  0.00           H
ATOM   1299 3HE  MET   201      33.656   2.694  27.230  1.00  0.00           H
ATOM   1300  N   ARG   202      35.975   7.374  30.873  1.00  0.00           N
ATOM   1301  CA  ARG   202      36.676   7.778  32.060  1.00  0.00           C
ATOM   1302  C   ARG   202      36.273   9.176  32.395  1.00  0.00           C
ATOM   1303  O   ARG   202      35.972   9.491  33.545  1.00  0.00           O
ATOM   1304  CB  ARG   202      38.197   7.887  31.873  1.00  0.00           C
ATOM   1305  CG  ARG   202      38.943   6.593  31.561  1.00  0.00           C
ATOM   1306  CD  ARG   202      40.437   6.852  31.353  1.00  0.00           C
ATOM   1307  NE  ARG   202      41.109   5.558  31.053  1.00  0.00           N
ATOM   1308  CZ  ARG   202      41.993   5.490  30.016  1.00  0.00           C
ATOM   1309 NH1  ARG   202      42.188   6.583  29.219  1.00  0.00           N
ATOM   1310 NH2  ARG   202      42.678   4.335  29.770  1.00  0.00           N
ATOM   1311  H   ARG   202      36.501   7.118  30.025  1.00  0.00           H
ATOM   1312  HA  ARG   202      36.405   7.099  32.869  1.00  0.00           H
ATOM   1313 1HB  ARG   202      38.617   8.277  32.799  1.00  0.00           H
ATOM   1314 2HB  ARG   202      38.380   8.565  31.040  1.00  0.00           H
ATOM   1315 1HG  ARG   202      38.558   6.125  30.654  1.00  0.00           H
ATOM   1316 2HG  ARG   202      38.841   5.873  32.373  1.00  0.00           H
ATOM   1317 1HD  ARG   202      40.846   7.286  32.264  1.00  0.00           H
ATOM   1318 2HD  ARG   202      40.559   7.542  30.518  1.00  0.00           H
ATOM   1319  HE  ARG   202      40.908   4.723  31.622  1.00  0.00           H
ATOM   1320 1HH1 ARG   202      41.668   7.453  29.402  1.00  0.00           H
ATOM   1321 2HH1 ARG   202      42.854   6.536  28.435  1.00  0.00           H
ATOM   1322 1HH2 ARG   202      42.528   3.510  30.368  1.00  0.00           H
ATOM   1323 2HH2 ARG   202      43.344   4.288  28.985  1.00  0.00           H
ATOM   1324  N   MET   203      36.247  10.050  31.374  1.00  0.00           N
ATOM   1325  CA  MET   203      36.017  11.448  31.587  1.00  0.00           C
ATOM   1326  C   MET   203      34.664  11.639  32.181  1.00  0.00           C
ATOM   1327  O   MET   203      34.483  12.426  33.106  1.00  0.00           O
ATOM   1328  CB  MET   203      36.040  12.247  30.275  1.00  0.00           C
ATOM   1329  CG  MET   203      36.305  13.743  30.460  1.00  0.00           C
ATOM   1330  SD  MET   203      38.063  14.190  30.635  1.00  0.00           S
ATOM   1331  CE  MET   203      38.429  13.087  32.030  1.00  0.00           C
ATOM   1332  H   MET   203      36.396   9.706  30.414  1.00  0.00           H
ATOM   1333  HA  MET   203      36.774  11.837  32.267  1.00  0.00           H
ATOM   1334 1HB  MET   203      35.069  12.138  29.790  1.00  0.00           H
ATOM   1335 2HB  MET   203      36.831  11.845  29.642  1.00  0.00           H
ATOM   1336 1HG  MET   203      35.791  14.070  31.364  1.00  0.00           H
ATOM   1337 2HG  MET   203      35.918  14.267  29.586  1.00  0.00           H
ATOM   1338 1HE  MET   203      37.528  12.537  32.305  1.00  0.00           H
ATOM   1339 2HE  MET   203      39.210  12.383  31.742  1.00  0.00           H
ATOM   1340 3HE  MET   203      38.767  13.677  32.881  1.00  0.00           H
ATOM   1341  N   LYS   204      33.657  10.928  31.660  1.00  0.00           N
ATOM   1342  CA  LYS   204      32.345  11.162  32.170  1.00  0.00           C
ATOM   1343  C   LYS   204      32.172  10.597  33.542  1.00  0.00           C
ATOM   1344  O   LYS   204      31.300  11.030  34.287  1.00  0.00           O
ATOM   1345  CB  LYS   204      31.205  10.660  31.289  1.00  0.00           C
ATOM   1346  CG  LYS   204      29.883  11.352  31.643  1.00  0.00           C
ATOM   1347  CD  LYS   204      29.808  12.801  31.166  1.00  0.00           C
ATOM   1348  CE  LYS   204      29.989  12.939  29.654  1.00  0.00           C
ATOM   1349  NZ  LYS   204      29.112  11.989  28.941  1.00  0.00           N
ATOM   1350  H   LYS   204      33.823  10.235  30.916  1.00  0.00           H
ATOM   1351  HA  LYS   204      32.117  12.226  32.233  1.00  0.00           H
ATOM   1352 1HB  LYS   204      31.057   9.586  31.407  1.00  0.00           H
ATOM   1353 2HB  LYS   204      31.406  10.851  30.235  1.00  0.00           H
ATOM   1354 1HG  LYS   204      29.688  11.393  32.714  1.00  0.00           H
ATOM   1355 2HG  LYS   204      29.008  10.864  31.212  1.00  0.00           H
```

```
ATOM   1356 1HD  LYS  204      30.571  13.435  31.616  1.00  0.00           H
ATOM   1357 2HD  LYS  204      28.853  13.273  31.396  1.00  0.00           H
ATOM   1358 1HE  LYS  204      31.022  12.732  29.374  1.00  0.00           H
ATOM   1359 2HE  LYS  204      29.738  13.949  29.331  1.00  0.00           H
ATOM   1360 1HZ  LYS  204      28.570  11.441  29.624  1.00  0.00           H
ATOM   1361 2HZ  LYS  204      28.466  12.509  28.329  1.00  0.00           H
ATOM   1362 3HZ  LYS  204      29.686  11.352  28.370  1.00  0.00           H
ATOM   1363  N   THR  205      32.937   9.558  33.895  1.00  0.00           N
ATOM   1364  CA  THR  205      32.820   8.959  35.191  1.00  0.00           C
ATOM   1365  C   THR  205      33.421   9.841  36.234  1.00  0.00           C
ATOM   1366  O   THR  205      33.103   9.701  37.413  1.00  0.00           O
ATOM   1367  CB  THR  205      33.476   7.622  35.274  1.00  0.00           C
ATOM   1368  OG1 THR  205      34.878   7.724  35.072  1.00  0.00           O
ATOM   1369  CG2 THR  205      32.847   6.772  34.170  1.00  0.00           C
ATOM   1370  H   THR  205      33.621   9.182  33.223  1.00  0.00           H
ATOM   1371  HA  THR  205      31.772   8.793  35.444  1.00  0.00           H
ATOM   1372  HB  THR  205      33.259   7.240  36.271  1.00  0.00           H
ATOM   1373  HG1 THR  205      35.287   8.327  35.799  1.00  0.00           H
ATOM   1374 1HG2 THR  205      32.105   7.363  33.633  1.00  0.00           H
ATOM   1375 2HG2 THR  205      33.621   6.445  33.476  1.00  0.00           H
ATOM   1376 3HG2 THR  205      32.365   5.899  34.612  1.00  0.00           H
ATOM   1377  N   ILE  206      34.329  10.754  35.842  1.00  0.00           N
ATOM   1378  CA  ILE  206      35.034  11.535  36.816  1.00  0.00           C
ATOM   1379  C   ILE  206      34.105  12.396  37.621  1.00  0.00           C
ATOM   1380  O   ILE  206      34.317  12.542  38.819  1.00  0.00           O
ATOM   1381  CB  ILE  206      36.137  12.392  36.249  1.00  0.00           C
ATOM   1382  CG1 ILE  206      35.624  13.519  35.338  1.00  0.00           C
ATOM   1383  CG2 ILE  206      37.115  11.439  35.546  1.00  0.00           C
ATOM   1384  CD1 ILE  206      35.054  14.729  36.079  1.00  0.00           C
ATOM   1385  H   ILE  206      34.518  10.892  34.838  1.00  0.00           H
ATOM   1386  HA  ILE  206      35.578  10.908  37.522  1.00  0.00           H
ATOM   1387  HB  ILE  206      36.597  12.905  37.093  1.00  0.00           H
ATOM   1388 1HG1 ILE  206      34.830  13.114  34.710  1.00  0.00           H
ATOM   1389 2HG1 ILE  206      36.456  13.869  34.728  1.00  0.00           H
ATOM   1390 1HG2 ILE  206      36.757  10.414  35.642  1.00  0.00           H
ATOM   1391 2HG2 ILE  206      37.183  11.701  34.490  1.00  0.00           H
ATOM   1392 3HG2 ILE  206      38.099  11.524  36.005  1.00  0.00           H
ATOM   1393 1HD1 ILE  206      35.119  14.561  37.154  1.00  0.00           H
ATOM   1394 2HD1 ILE  206      35.624  15.619  35.815  1.00  0.00           H
ATOM   1395 3HD1 ILE  206      34.010  14.870  35.797  1.00  0.00           H
ATOM   1396  N   GLY  207      33.051  12.996  37.034  1.00  0.00           N
ATOM   1397  CA  GLY  207      32.264  13.845  37.883  1.00  0.00           C
ATOM   1398  C   GLY  207      30.833  13.516  37.728  1.00  0.00           C
ATOM   1399  O   GLY  207      30.434  12.850  36.776  1.00  0.00           O
ATOM   1400  H   GLY  207      32.824  12.854  36.039  1.00  0.00           H
ATOM   1401 1HA  GLY  207      32.424  14.888  37.610  1.00  0.00           H
ATOM   1402 2HA  GLY  207      32.555  13.697  38.922  1.00  0.00           H
ATOM   1403  N   GLU  208      30.014  13.978  38.690  1.00  0.00           N
ATOM   1404  CA  GLU  208      28.631  13.734  38.496  1.00  0.00           C
ATOM   1405  C   GLU  208      28.284  14.781  37.488  1.00  0.00           C
ATOM   1406  O   GLU  208      27.981  15.916  37.843  1.00  0.00           O
ATOM   1407  CB  GLU  208      27.794  13.968  39.758  1.00  0.00           C
ATOM   1408  CG  GLU  208      28.261  13.090  40.923  1.00  0.00           C
ATOM   1409  CD  GLU  208      28.611  11.716  40.364  1.00  0.00           C
ATOM   1410  OE1 GLU  208      27.837  11.214  39.505  1.00  0.00           O
ATOM   1411  OE2 GLU  208      29.656  11.152  40.786  1.00  0.00           O
ATOM   1412  H   GLU  208      30.369  14.478  39.516  1.00  0.00           H
ATOM   1413  HA  GLU  208      28.451  12.723  38.128  1.00  0.00           H
ATOM   1414 1HB  GLU  208      26.740  13.744  39.593  1.00  0.00           H
ATOM   1415 2HB  GLU  208      27.850  15.002  40.096  1.00  0.00           H
ATOM   1416 1HG  GLU  208      27.443  13.022  41.640  1.00  0.00           H
ATOM   1417 2HG  GLU  208      29.135  13.563  41.370  1.00  0.00           H
ATOM   1418  N   HIS  209      28.353  14.427  36.189  1.00  0.00           N
ATOM   1419  CA  HIS  209      28.205  15.402  35.146  1.00  0.00           C
ATOM   1420  C   HIS  209      26.837  15.990  35.084  1.00  0.00           C
ATOM   1421  O   HIS  209      26.701  17.181  34.811  1.00  0.00           O
ATOM   1422  CB  HIS  209      28.616  14.926  33.740  1.00  0.00           C
ATOM   1423  CG  HIS  209      30.061  15.227  33.463  1.00  0.00           C
```

```
ATOM   1424  ND1 HIS   209      30.499  16.447  32.996  1.00  0.00           N
ATOM   1425  CD2 HIS   209      31.178  14.464  33.616  1.00  0.00           C
ATOM   1426  CE1 HIS   209      31.847  16.367  32.896  1.00  0.00           C
ATOM   1427  NE2 HIS   209      32.306  15.182  33.258  1.00  0.00           N
ATOM   1428  H   HIS   209      28.514  13.440  35.940  1.00  0.00           H
ATOM   1429  HA  HIS   209      28.883  16.248  35.252  1.00  0.00           H
ATOM   1430 1HB  HIS   209      28.023  15.415  32.967  1.00  0.00           H
ATOM   1431 2HB  HIS   209      28.476  13.850  33.629  1.00  0.00           H
ATOM   1432  HD1 HIS   209      29.913  17.263  32.767  1.00  0.00           H
ATOM   1433  HD2 HIS   209      31.183  13.433  33.970  1.00  0.00           H
ATOM   1434  HE1 HIS   209      32.480  17.186  32.555  1.00  0.00           H
ATOM   1435  HE2 HIS   209      33.285  14.863  33.270  1.00  0.00           H
ATOM   1436  N   ILE   210      25.788  15.189  35.333  1.00  0.00           N
ATOM   1437  CA  ILE   210      24.456  15.709  35.250  1.00  0.00           C
ATOM   1438  C   ILE   210      24.317  16.825  36.239  1.00  0.00           C
ATOM   1439  O   ILE   210      23.712  17.852  35.936  1.00  0.00           O
ATOM   1440  CB  ILE   210      23.410  14.681  35.589  1.00  0.00           C
ATOM   1441  CG1 ILE   210      23.451  13.504  34.604  1.00  0.00           C
ATOM   1442  CG2 ILE   210      22.049  15.384  35.643  1.00  0.00           C
ATOM   1443  CD1 ILE   210      22.594  12.326  35.062  1.00  0.00           C
ATOM   1444  H   ILE   210      25.941  14.201  35.583  1.00  0.00           H
ATOM   1445  HA  ILE   210      24.289  16.076  34.237  1.00  0.00           H
ATOM   1446  HB  ILE   210      23.660  14.248  36.557  1.00  0.00           H
ATOM   1447 1HG1 ILE   210      24.457  13.110  34.463  1.00  0.00           H
ATOM   1448 2HG1 ILE   210      23.089  13.775  33.612  1.00  0.00           H
ATOM   1449 1HG2 ILE   210      22.178  16.444  35.424  1.00  0.00           H
ATOM   1450 2HG2 ILE   210      21.380  14.940  34.905  1.00  0.00           H
ATOM   1451 3HG2 ILE   210      21.619  15.268  36.638  1.00  0.00           H
ATOM   1452 1HD1 ILE   210      22.120  12.568  36.013  1.00  0.00           H
ATOM   1453 2HD1 ILE   210      21.826  12.122  34.315  1.00  0.00           H
ATOM   1454 3HD1 ILE   210      23.223  11.444  35.184  1.00  0.00           H
ATOM   1455  N   VAL   211      24.869  16.664  37.456  1.00  0.00           N
ATOM   1456  CA  VAL   211      24.693  17.704  38.431  1.00  0.00           C
ATOM   1457  C   VAL   211      25.417  18.932  37.989  1.00  0.00           C
ATOM   1458  O   VAL   211      24.936  20.045  38.195  1.00  0.00           O
ATOM   1459  CB  VAL   211      25.127  17.349  39.819  1.00  0.00           C
ATOM   1460  CG1 VAL   211      24.270  16.147  40.226  1.00  0.00           C
ATOM   1461  CG2 VAL   211      26.648  17.145  39.891  1.00  0.00           C
ATOM   1462  H   VAL   211      25.405  15.814  37.683  1.00  0.00           H
ATOM   1463  HA  VAL   211      23.631  17.929  38.537  1.00  0.00           H
ATOM   1464  HB  VAL   211      24.932  18.234  40.424  1.00  0.00           H
ATOM   1465 1HG1 VAL   211      23.595  15.888  39.409  1.00  0.00           H
ATOM   1466 2HG1 VAL   211      24.916  15.297  40.446  1.00  0.00           H
ATOM   1467 3HG1 VAL   211      23.687  16.398  41.112  1.00  0.00           H
ATOM   1468 1HG2 VAL   211      27.083  17.305  38.904  1.00  0.00           H
ATOM   1469 2HG2 VAL   211      27.077  17.855  40.597  1.00  0.00           H
ATOM   1470 3HG2 VAL   211      26.863  16.129  40.222  1.00  0.00           H
ATOM   1471  N   ALA   212      26.600  18.777  37.366  1.00  0.00           N
ATOM   1472  CA  ALA   212      27.310  19.959  36.980  1.00  0.00           C
ATOM   1473  C   ALA   212      26.495  20.728  35.979  1.00  0.00           C
ATOM   1474  O   ALA   212      26.306  21.937  36.114  1.00  0.00           O
ATOM   1475  CB  ALA   212      28.679  19.661  36.344  1.00  0.00           C
ATOM   1476  H   ALA   212      26.981  17.839  37.173  1.00  0.00           H
ATOM   1477  HA  ALA   212      27.486  20.579  37.858  1.00  0.00           H
ATOM   1478 1HB  ALA   212      28.839  18.583  36.313  1.00  0.00           H
ATOM   1479 2HB  ALA   212      28.703  20.060  35.330  1.00  0.00           H
ATOM   1480 3HB  ALA   212      29.465  20.127  36.937  1.00  0.00           H
ATOM   1481  N   HIS   213      25.966  20.037  34.952  1.00  0.00           N
ATOM   1482  CA  HIS   213      25.230  20.689  33.902  1.00  0.00           C
ATOM   1483  C   HIS   213      23.947  21.271  34.410  1.00  0.00           C
ATOM   1484  O   HIS   213      23.565  22.378  34.030  1.00  0.00           O
ATOM   1485  CB  HIS   213      24.836  19.741  32.759  1.00  0.00           C
ATOM   1486  CG  HIS   213      25.993  19.281  31.927  1.00  0.00           C
ATOM   1487  ND1 HIS   213      25.864  18.426  30.856  1.00  0.00           N
ATOM   1488  CD2 HIS   213      27.319  19.575  32.011  1.00  0.00           C
ATOM   1489  CE1 HIS   213      27.108  18.249  30.345  1.00  0.00           C
ATOM   1490  NE2 HIS   213      28.025  18.926  31.013  1.00  0.00           N
ATOM   1491  H   HIS   213      26.091  19.015  34.917  1.00  0.00           H
```

```
ATOM   1492  HA  HIS  213      25.802  21.503  33.458  1.00  0.00           H
ATOM   1493 1HB  HIS  213      24.140  20.263  32.102  1.00  0.00           H
ATOM   1494 2HB  HIS  213      24.364  18.858  33.191  1.00  0.00           H
ATOM   1495  HD1 HIS  213      24.991  18.002  30.509  1.00  0.00           H
ATOM   1496  HD2 HIS  213      27.763  20.230  32.760  1.00  0.00           H
ATOM   1497  HE1 HIS  213      27.326  17.620  29.481  1.00  0.00           H
ATOM   1498  HE2 HIS  213      29.038  18.962  30.831  1.00  0.00           H
ATOM   1499  N   ILE  214      23.233  20.532  35.275  1.00  0.00           N
ATOM   1500  CA  ILE  214      21.952  20.991  35.725  1.00  0.00           C
ATOM   1501  C   ILE  214      22.133  22.235  36.526  1.00  0.00           C
ATOM   1502  O   ILE  214      21.288  23.128  36.492  1.00  0.00           O
ATOM   1503  CB  ILE  214      21.221  20.006  36.587  1.00  0.00           C
ATOM   1504  CG1 ILE  214      21.026  18.672  35.855  1.00  0.00           C
ATOM   1505  CG2 ILE  214      19.879  20.645  36.977  1.00  0.00           C
ATOM   1506  CD1 ILE  214      20.453  17.586  36.763  1.00  0.00           C
ATOM   1507  H   ILE  214      23.606  19.634  35.615  1.00  0.00           H
ATOM   1508  HA  ILE  214      21.322  21.197  34.859  1.00  0.00           H
ATOM   1509  HB  ILE  214      21.842  19.815  37.462  1.00  0.00           H
ATOM   1510 1HG1 ILE  214      21.959  18.275  35.455  1.00  0.00           H
ATOM   1511 2HG1 ILE  214      20.342  18.756  35.010  1.00  0.00           H
ATOM   1512 1HG2 ILE  214      19.805  21.637  36.531  1.00  0.00           H
ATOM   1513 2HG2 ILE  214      19.060  20.023  36.614  1.00  0.00           H
ATOM   1514 3HG2 ILE  214      19.817  20.728  38.062  1.00  0.00           H
ATOM   1515 1HD1 ILE  214      20.298  17.991  37.762  1.00  0.00           H
ATOM   1516 2HD1 ILE  214      19.500  17.240  36.360  1.00  0.00           H
ATOM   1517 3HD1 ILE  214      21.150  16.749  36.814  1.00  0.00           H
ATOM   1518  N   GLN  215      23.248  22.330  37.270  1.00  0.00           N
ATOM   1519  CA  GLN  215      23.456  23.479  38.098  1.00  0.00           C
ATOM   1520  C   GLN  215      23.439  24.675  37.208  1.00  0.00           C
ATOM   1521  O   GLN  215      22.818  25.688  37.526  1.00  0.00           O
ATOM   1522  CB  GLN  215      24.809  23.448  38.840  1.00  0.00           C
ATOM   1523  CG  GLN  215      25.064  24.664  39.737  1.00  0.00           C
ATOM   1524  CD  GLN  215      25.576  25.823  38.890  1.00  0.00           C
ATOM   1525  OE1 GLN  215      25.486  26.981  39.294  1.00  0.00           O
ATOM   1526  NE2 GLN  215      26.139  25.506  37.693  1.00  0.00           N
ATOM   1527  H   GLN  215      23.951  21.577  37.244  1.00  0.00           H
ATOM   1528  HA  GLN  215      22.642  23.507  38.822  1.00  0.00           H
ATOM   1529 1HB  GLN  215      25.605  23.411  38.097  1.00  0.00           H
ATOM   1530 2HB  GLN  215      24.832  22.560  39.471  1.00  0.00           H
ATOM   1531 1HG  GLN  215      25.808  24.410  40.491  1.00  0.00           H
ATOM   1532 2HG  GLN  215      24.135  24.955  40.227  1.00  0.00           H
ATOM   1533 1HE2 GLN  215      26.510  26.250  37.085  1.00  0.00           H
ATOM   1534 2HE2 GLN  215      26.193  24.521  37.394  1.00  0.00           H
ATOM   1535  N   HIS  216      24.099  24.574  36.042  1.00  0.00           N
ATOM   1536  CA  HIS  216      24.140  25.700  35.162  1.00  0.00           C
ATOM   1537  C   HIS  216      22.738  26.055  34.766  1.00  0.00           C
ATOM   1538  O   HIS  216      22.360  27.225  34.780  1.00  0.00           O
ATOM   1539  CB  HIS  216      24.936  25.429  33.871  1.00  0.00           C
ATOM   1540  CG  HIS  216      26.420  25.354  34.086  1.00  0.00           C
ATOM   1541  ND1 HIS  216      27.091  24.230  34.514  1.00  0.00           N
ATOM   1542  CD2 HIS  216      27.373  26.311  33.914  1.00  0.00           C
ATOM   1543  CE1 HIS  216      28.406  24.559  34.579  1.00  0.00           C
ATOM   1544  NE2 HIS  216      28.626  25.812  34.223  1.00  0.00           N
ATOM   1545  H   HIS  216      24.570  23.694  35.785  1.00  0.00           H
ATOM   1546  HA  HIS  216      24.605  26.536  35.683  1.00  0.00           H
ATOM   1547 1HB  HIS  216      24.798  26.193  33.105  1.00  0.00           H
ATOM   1548 2HB  HIS  216      24.671  24.489  33.385  1.00  0.00           H
ATOM   1549  HD1 HIS  216      26.674  23.315  34.741  1.00  0.00           H
ATOM   1550  HD2 HIS  216      27.176  27.329  33.579  1.00  0.00           H
ATOM   1551  HE1 HIS  216      29.190  23.868  34.889  1.00  0.00           H
ATOM   1552  HE2 HIS  216      29.528  26.306  34.184  1.00  0.00           H
ATOM   1553  N   GLU  217      21.919  25.045  34.418  1.00  0.00           N
ATOM   1554  CA  GLU  217      20.587  25.304  33.946  1.00  0.00           C
ATOM   1555  C   GLU  217      19.754  25.956  35.006  1.00  0.00           C
ATOM   1556  O   GLU  217      19.127  26.983  34.752  1.00  0.00           O
ATOM   1557  CB  GLU  217      19.838  24.022  33.548  1.00  0.00           C
ATOM   1558  CG  GLU  217      20.439  23.309  32.340  1.00  0.00           C
ATOM   1559  CD  GLU  217      19.599  22.072  32.051  1.00  0.00           C
```

ATOM	1560	OE1	GLU	217	19.277	21.335	33.021	1.00	0.00	O
ATOM	1561	OE2	GLU	217	19.267	21.845	30.856	1.00	0.00	O
ATOM	1562	H	GLU	217	22.251	24.073	34.491	1.00	0.00	H
ATOM	1563	HA	GLU	217	20.597	25.965	33.079	1.00	0.00	H
ATOM	1564	1HB	GLU	217	18.793	24.187	33.284	1.00	0.00	H
ATOM	1565	2HB	GLU	217	19.811	23.267	34.333	1.00	0.00	H
ATOM	1566	1HG	GLU	217	21.464	23.030	32.584	1.00	0.00	H
ATOM	1567	2HG	GLU	217	20.417	23.995	31.493	1.00	0.00	H
ATOM	1568	N	VAL	218	19.761	25.387	36.228	1.00	0.00	N
ATOM	1569	CA	VAL	218	18.946	25.841	37.325	1.00	0.00	C
ATOM	1570	C	VAL	218	17.557	26.178	36.853	1.00	0.00	C
ATOM	1571	O	VAL	218	17.279	27.310	36.461	1.00	0.00	O
ATOM	1572	CB	VAL	218	19.537	27.001	38.086	1.00	0.00	C
ATOM	1573	CG1	VAL	218	19.787	28.182	37.131	1.00	0.00	C
ATOM	1574	CG2	VAL	218	18.595	27.337	39.254	1.00	0.00	C
ATOM	1575	H	VAL	218	20.384	24.582	36.386	1.00	0.00	H
ATOM	1576	HA	VAL	218	18.867	25.070	38.091	1.00	0.00	H
ATOM	1577	HB	VAL	218	20.482	26.704	38.539	1.00	0.00	H
ATOM	1578	1HG1	VAL	218	19.478	27.906	36.122	1.00	0.00	H
ATOM	1579	2HG1	VAL	218	19.211	29.046	37.462	1.00	0.00	H
ATOM	1580	3HG1	VAL	218	20.848	28.430	37.130	1.00	0.00	H
ATOM	1581	1HG2	VAL	218	17.742	26.658	39.240	1.00	0.00	H
ATOM	1582	2HG2	VAL	218	19.130	27.227	40.196	1.00	0.00	H
ATOM	1583	3HG2	VAL	218	18.243	28.363	39.153	1.00	0.00	H
ATOM	1584	N	ASP	219	16.632	25.186	36.896	1.00	0.00	N
ATOM	1585	CA	ASP	219	15.285	25.411	36.422	1.00	0.00	C
ATOM	1586	C	ASP	219	14.295	24.575	37.206	1.00	0.00	C
ATOM	1587	O	ASP	219	14.647	23.982	38.225	1.00	0.00	O
ATOM	1588	CB	ASP	219	15.116	25.023	34.944	1.00	0.00	C
ATOM	1589	CG	ASP	219	15.806	26.077	34.089	1.00	0.00	C
ATOM	1590	OD1	ASP	219	15.722	27.280	34.453	1.00	0.00	O
ATOM	1591	OD2	ASP	219	16.430	25.693	33.063	1.00	0.00	O
ATOM	1592	H	ASP	219	16.892	24.262	37.270	1.00	0.00	H
ATOM	1593	HA	ASP	219	15.008	26.459	36.532	1.00	0.00	H
ATOM	1594	1HB	ASP	219	14.050	24.985	34.718	1.00	0.00	H
ATOM	1595	2HB	ASP	219	15.574	24.046	34.790	1.00	0.00	H
ATOM	1596	N	PHE	220	13.010	24.525	36.743	1.00	0.00	N
ATOM	1597	CA	PHE	220	11.964	23.735	37.359	1.00	0.00	C
ATOM	1598	C	PHE	220	12.327	22.298	37.204	1.00	0.00	C
ATOM	1599	O	PHE	220	13.502	21.949	37.134	1.00	0.00	O
ATOM	1600	CB	PHE	220	10.563	23.849	36.720	1.00	0.00	C
ATOM	1601	CG	PHE	220	9.831	25.056	37.198	1.00	0.00	C
ATOM	1602	CD1	PHE	220	9.388	25.119	38.500	1.00	0.00	C
ATOM	1603	CD2	PHE	220	9.535	26.093	36.344	1.00	0.00	C
ATOM	1604	CE1	PHE	220	8.696	26.216	38.955	1.00	0.00	C
ATOM	1605	CE2	PHE	220	8.842	27.193	36.793	1.00	0.00	C
ATOM	1606	CZ	PHE	220	8.425	27.257	38.101	1.00	0.00	C
ATOM	1607	H	PHE	220	12.772	25.080	35.908	1.00	0.00	H
ATOM	1608	HA	PHE	220	11.910	24.014	38.411	1.00	0.00	H
ATOM	1609	1HB	PHE	220	9.939	22.986	36.952	1.00	0.00	H
ATOM	1610	2HB	PHE	220	10.616	23.919	35.633	1.00	0.00	H
ATOM	1611	HD1	PHE	220	9.588	24.289	39.177	1.00	0.00	H
ATOM	1612	HD2	PHE	220	9.852	26.042	35.302	1.00	0.00	H
ATOM	1613	HE1	PHE	220	8.362	26.259	39.991	1.00	0.00	H
ATOM	1614	HE2	PHE	220	8.623	28.014	36.110	1.00	0.00	H
ATOM	1615	HZ	PHE	220	7.881	28.130	38.459	1.00	0.00	H
ATOM	1616	N	LEU	221	11.300	21.423	37.148	1.00	0.00	N
ATOM	1617	CA	LEU	221	11.526	20.012	37.009	1.00	0.00	C
ATOM	1618	C	LEU	221	12.371	19.845	35.793	1.00	0.00	C
ATOM	1619	O	LEU	221	12.331	20.695	34.908	1.00	0.00	O
ATOM	1620	CB	LEU	221	10.240	19.203	36.758	1.00	0.00	C
ATOM	1621	CG	LEU	221	9.188	19.334	37.871	1.00	0.00	C
ATOM	1622	CD1	LEU	221	8.666	20.776	37.969	1.00	0.00	C
ATOM	1623	CD2	LEU	221	8.055	18.312	37.689	1.00	0.00	C
ATOM	1624	H	LEU	221	10.333	21.775	37.206	1.00	0.00	H
ATOM	1625	HA	LEU	221	12.035	19.695	37.919	1.00	0.00	H
ATOM	1626	1HB	LEU	221	10.507	18.149	36.676	1.00	0.00	H
ATOM	1627	2HB	LEU	221	9.788	19.556	35.831	1.00	0.00	H

ATOM	1628	HG	LEU	221	9.608	19.063	38.839	1.00	0.00	H
ATOM	1629	1HD1	LEU	221	9.161	21.394	37.220	1.00	0.00	H
ATOM	1630	2HD1	LEU	221	7.590	20.786	37.793	1.00	0.00	H
ATOM	1631	3HD1	LEU	221	8.875	21.172	38.962	1.00	0.00	H
ATOM	1632	1HD2	LEU	221	8.246	17.710	36.800	1.00	0.00	H
ATOM	1633	2HD2	LEU	221	8.006	17.662	38.563	1.00	0.00	H
ATOM	1634	3HD2	LEU	221	7.106	18.836	37.574	1.00	0.00	H
ATOM	1635	N	PHE	222	13.170	18.758	35.719	1.00	0.00	N
ATOM	1636	CA	PHE	222	14.012	18.591	34.568	1.00	0.00	C
ATOM	1637	C	PHE	222	13.954	17.178	34.077	1.00	0.00	C
ATOM	1638	O	PHE	222	13.414	16.287	34.732	1.00	0.00	O
ATOM	1639	CB	PHE	222	15.491	18.954	34.813	1.00	0.00	C
ATOM	1640	CG	PHE	222	16.042	18.085	35.894	1.00	0.00	C
ATOM	1641	CD1	PHE	222	15.894	18.442	37.214	1.00	0.00	C
ATOM	1642	CD2	PHE	222	16.713	16.922	35.590	1.00	0.00	C
ATOM	1643	CE1	PHE	222	16.404	17.652	38.216	1.00	0.00	C
ATOM	1644	CE2	PHE	222	17.225	16.126	36.589	1.00	0.00	C
ATOM	1645	CZ	PHE	222	17.071	16.492	37.904	1.00	0.00	C
ATOM	1646	H	PHE	222	13.175	18.060	36.476	1.00	0.00	H
ATOM	1647	HA	PHE	222	13.690	19.249	33.761	1.00	0.00	H
ATOM	1648	1HB	PHE	222	15.562	19.999	35.113	1.00	0.00	H
ATOM	1649	2HB	PHE	222	16.058	18.798	33.895	1.00	0.00	H
ATOM	1650	HD1	PHE	222	15.366	19.361	37.468	1.00	0.00	H
ATOM	1651	HD2	PHE	222	16.840	16.628	34.547	1.00	0.00	H
ATOM	1652	HE1	PHE	222	16.279	17.945	39.258	1.00	0.00	H
ATOM	1653	HE2	PHE	222	17.752	15.205	36.337	1.00	0.00	H
ATOM	1654	HZ	PHE	222	17.476	15.864	38.697	1.00	0.00	H
ATOM	1655	N	CYS	223	14.495	16.954	32.860	1.00	0.00	N
ATOM	1656	CA	CYS	223	14.523	15.645	32.272	1.00	0.00	C
ATOM	1657	C	CYS	223	15.892	15.430	31.711	1.00	0.00	C
ATOM	1658	O	CYS	223	16.741	16.317	31.765	1.00	0.00	O
ATOM	1659	CB	CYS	223	13.513	15.449	31.131	1.00	0.00	C
ATOM	1660	SG	CYS	223	11.804	15.347	31.734	1.00	0.00	S
ATOM	1661	H	CYS	223	14.899	17.745	32.338	1.00	0.00	H
ATOM	1662	HA	CYS	223	14.301	14.924	33.059	1.00	0.00	H
ATOM	1663	1HB	CYS	223	13.697	14.534	30.567	1.00	0.00	H
ATOM	1664	2HB	CYS	223	13.538	16.266	30.410	1.00	0.00	H
ATOM	1665	HG	CYS	223	11.311	16.583	31.894	1.00	0.00	H
ATOM	1666	N	MET	224	16.151	14.223	31.171	1.00	0.00	N
ATOM	1667	CA	MET	224	17.462	13.955	30.656	1.00	0.00	C
ATOM	1668	C	MET	224	17.336	13.567	29.227	1.00	0.00	C
ATOM	1669	O	MET	224	16.274	13.636	28.638	1.00	0.00	O
ATOM	1670	CB	MET	224	18.205	12.807	31.356	1.00	0.00	C
ATOM	1671	CG	MET	224	18.579	13.131	32.805	1.00	0.00	C
ATOM	1672	SD	MET	224	19.743	11.963	33.559	1.00	0.00	S
ATOM	1673	CE	MET	224	21.132	12.454	32.499	1.00	0.00	C
ATOM	1674	H	MET	224	15.416	13.502	31.128	1.00	0.00	H
ATOM	1675	HA	MET	224	18.062	14.859	30.753	1.00	0.00	H
ATOM	1676	1HB	MET	224	19.139	12.540	30.862	1.00	0.00	H
ATOM	1677	2HB	MET	224	17.622	11.886	31.400	1.00	0.00	H
ATOM	1678	1HG	MET	224	17.667	13.121	33.403	1.00	0.00	H
ATOM	1679	2HG	MET	224	19.041	14.117	32.825	1.00	0.00	H
ATOM	1680	1HE	MET	224	20.807	13.236	31.813	1.00	0.00	H
ATOM	1681	2HE	MET	224	21.947	12.828	33.117	1.00	0.00	H
ATOM	1682	3HE	MET	224	21.476	11.591	31.928	1.00	0.00	H
ATOM	1683	N	ASP	225	18.477	13.306	28.585	1.00	0.00	N
ATOM	1684	CA	ASP	225	18.574	12.743	27.269	1.00	0.00	C
ATOM	1685	C	ASP	225	18.441	11.266	27.412	1.00	0.00	C
ATOM	1686	O	ASP	225	17.947	10.561	26.527	1.00	0.00	O
ATOM	1687	CB	ASP	225	19.958	13.023	26.656	1.00	0.00	C
ATOM	1688	CG	ASP	225	21.036	12.366	27.527	1.00	0.00	C
ATOM	1689	OD1	ASP	225	20.926	12.417	28.783	1.00	0.00	O
ATOM	1690	OD2	ASP	225	21.989	11.795	26.930	1.00	0.00	O
ATOM	1691	H	ASP	225	19.357	13.526	29.072	1.00	0.00	H
ATOM	1692	HA	ASP	225	17.761	13.165	26.678	1.00	0.00	H
ATOM	1693	1HB	ASP	225	20.120	14.100	26.617	1.00	0.00	H
ATOM	1694	2HB	ASP	225	19.993	12.607	25.648	1.00	0.00	H
ATOM	1695	N	VAL	226	18.856	10.834	28.623	1.00	0.00	N

ATOM	1696	CA	VAL	226	19.158	9.502	29.031	1.00	0.00	C
ATOM	1697	C	VAL	226	18.347	8.518	28.280	1.00	0.00	C
ATOM	1698	O	VAL	226	18.884	7.845	27.398	1.00	0.00	O
ATOM	1699	CB	VAL	226	18.990	9.296	30.517	1.00	0.00	C
ATOM	1700	CG1	VAL	226	17.611	9.798	30.968	1.00	0.00	C
ATOM	1701	CG2	VAL	226	19.236	7.806	30.813	1.00	0.00	C
ATOM	1702	H	VAL	226	18.968	11.560	29.344	1.00	0.00	H
ATOM	1703	HA	VAL	226	20.208	9.267	28.859	1.00	0.00	H
ATOM	1704	HB	VAL	226	19.758	9.844	31.061	1.00	0.00	H
ATOM	1705	1HG1	VAL	226	17.067	10.189	30.108	1.00	0.00	H
ATOM	1706	2HG1	VAL	226	17.049	8.973	31.407	1.00	0.00	H
ATOM	1707	3HG1	VAL	226	17.735	10.587	31.708	1.00	0.00	H
ATOM	1708	1HG2	VAL	226	19.466	7.283	29.884	1.00	0.00	H
ATOM	1709	2HG2	VAL	226	20.073	7.705	31.503	1.00	0.00	H
ATOM	1710	3HG2	VAL	226	18.342	7.371	31.261	1.00	0.00	H
ATOM	1711	N	ASP	227	17.039	8.440	28.569	1.00	0.00	N
ATOM	1712	CA	ASP	227	16.309	7.427	27.888	1.00	0.00	C
ATOM	1713	C	ASP	227	14.967	7.350	28.528	1.00	0.00	C
ATOM	1714	O	ASP	227	14.329	6.298	28.509	1.00	0.00	O
ATOM	1715	CB	ASP	227	16.952	6.035	28.074	1.00	0.00	C
ATOM	1716	CG	ASP	227	17.128	5.778	29.562	1.00	0.00	C
ATOM	1717	OD1	ASP	227	17.242	6.775	30.322	1.00	0.00	O
ATOM	1718	OD2	ASP	227	17.127	4.585	29.966	1.00	0.00	O
ATOM	1719	H	ASP	227	16.590	9.075	29.243	1.00	0.00	H
ATOM	1720	HA	ASP	227	16.241	7.728	26.842	1.00	0.00	H
ATOM	1721	1HB	ASP	227	17.919	6.029	27.571	1.00	0.00	H
ATOM	1722	2HB	ASP	227	16.292	5.286	27.635	1.00	0.00	H
ATOM	1723	N	GLN	228	14.479	8.462	29.110	1.00	0.00	N
ATOM	1724	CA	GLN	228	13.185	8.299	29.701	1.00	0.00	C
ATOM	1725	C	GLN	228	12.303	9.423	29.286	1.00	0.00	C
ATOM	1726	O	GLN	228	12.746	10.488	28.871	1.00	0.00	O
ATOM	1727	CB	GLN	228	13.189	8.205	31.239	1.00	0.00	C
ATOM	1728	CG	GLN	228	13.694	9.436	31.978	1.00	0.00	C
ATOM	1729	CD	GLN	228	12.506	10.256	32.470	1.00	0.00	C
ATOM	1730	OE1	GLN	228	11.525	10.507	31.769	1.00	0.00	O
ATOM	1731	NE2	GLN	228	12.609	10.695	33.753	1.00	0.00	N
ATOM	1732	H	GLN	228	14.993	9.354	29.128	1.00	0.00	H
ATOM	1733	HA	GLN	228	12.749	7.356	29.370	1.00	0.00	H
ATOM	1734	1HB	GLN	228	13.834	7.373	31.522	1.00	0.00	H
ATOM	1735	2HB	GLN	228	12.163	8.032	31.566	1.00	0.00	H
ATOM	1736	1HG	GLN	228	14.299	10.041	31.303	1.00	0.00	H
ATOM	1737	2HG	GLN	228	14.299	9.125	32.829	1.00	0.00	H
ATOM	1738	1HE2	GLN	228	11.851	11.256	34.167	1.00	0.00	H
ATOM	1739	2HE2	GLN	228	13.444	10.465	34.310	1.00	0.00	H
ATOM	1740	N	VAL	229	10.985	9.216	29.302	1.00	0.00	N
ATOM	1741	CA	VAL	229	10.265	10.409	29.007	1.00	0.00	C
ATOM	1742	C	VAL	229	8.943	10.261	29.650	1.00	0.00	C
ATOM	1743	O	VAL	229	8.623	9.181	30.145	1.00	0.00	O
ATOM	1744	CB	VAL	229	10.113	10.706	27.554	1.00	0.00	C
ATOM	1745	CG1	VAL	229	8.812	10.093	27.020	1.00	0.00	C
ATOM	1746	CG2	VAL	229	10.297	12.218	27.396	1.00	0.00	C
ATOM	1747	H	VAL	229	10.543	8.307	29.502	1.00	0.00	H
ATOM	1748	HA	VAL	229	10.847	11.227	29.430	1.00	0.00	H
ATOM	1749	HB	VAL	229	10.950	10.289	26.994	1.00	0.00	H
ATOM	1750	1HG1	VAL	229	8.293	9.578	27.828	1.00	0.00	H
ATOM	1751	2HG1	VAL	229	8.173	10.882	26.624	1.00	0.00	H
ATOM	1752	3HG1	VAL	229	9.043	9.382	26.226	1.00	0.00	H
ATOM	1753	1HG2	VAL	229	10.486	12.665	28.371	1.00	0.00	H
ATOM	1754	2HG2	VAL	229	11.142	12.414	26.736	1.00	0.00	H
ATOM	1755	3HG2	VAL	229	9.393	12.651	26.967	1.00	0.00	H
ATOM	1756	N	PHE	230	8.137	11.336	29.699	1.00	0.00	N
ATOM	1757	CA	PHE	230	6.941	11.031	30.407	1.00	0.00	C
ATOM	1758	C	PHE	230	6.080	10.040	29.682	1.00	0.00	C
ATOM	1759	O	PHE	230	5.747	10.180	28.506	1.00	0.00	O
ATOM	1760	CB	PHE	230	6.180	12.166	31.153	1.00	0.00	C
ATOM	1761	CG	PHE	230	6.085	13.496	30.474	1.00	0.00	C
ATOM	1762	CD1	PHE	230	5.393	13.701	29.304	1.00	0.00	C
ATOM	1763	CD2	PHE	230	6.665	14.576	31.097	1.00	0.00	C

ATOM	1764	CE1	PHE	230	5.326	14.963	28.755	1.00	0.00	C
ATOM	1765	CE2	PHE	230	6.606	15.837	30.560	1.00	0.00	C
ATOM	1766	CZ	PHE	230	5.934	16.030	29.377	1.00	0.00	C
ATOM	1767	H	PHE	230	8.354	12.252	29.282	1.00	0.00	H
ATOM	1768	HA	PHE	230	7.134	10.603	31.390	1.00	0.00	H
ATOM	1769	1HB	PHE	230	6.692	12.337	32.099	1.00	0.00	H
ATOM	1770	2HB	PHE	230	5.156	11.825	31.311	1.00	0.00	H
ATOM	1771	HD1	PHE	230	4.897	12.865	28.810	1.00	0.00	H
ATOM	1772	HD2	PHE	230	7.185	14.426	32.042	1.00	0.00	H
ATOM	1773	HE1	PHE	230	4.787	15.117	27.820	1.00	0.00	H
ATOM	1774	HE2	PHE	230	7.086	16.675	31.065	1.00	0.00	H
ATOM	1775	HZ	PHE	230	5.882	17.024	28.932	1.00	0.00	H
ATOM	1776	N	GLN	231	5.783	8.965	30.445	1.00	0.00	N
ATOM	1777	CA	GLN	231	5.096	7.740	30.141	1.00	0.00	C
ATOM	1778	C	GLN	231	3.686	8.004	29.740	1.00	0.00	C
ATOM	1779	O	GLN	231	3.205	7.413	28.775	1.00	0.00	O
ATOM	1780	CB	GLN	231	5.053	6.853	31.396	1.00	0.00	C
ATOM	1781	CG	GLN	231	4.363	5.498	31.242	1.00	0.00	C
ATOM	1782	CD	GLN	231	4.308	4.877	32.635	1.00	0.00	C
ATOM	1783	OE1	GLN	231	3.298	4.306	33.045	1.00	0.00	O
ATOM	1784	NE2	GLN	231	5.432	4.995	33.394	1.00	0.00	N
ATOM	1785	H	GLN	231	6.107	9.036	31.420	1.00	0.00	H
ATOM	1786	HA	GLN	231	5.583	7.211	29.322	1.00	0.00	H
ATOM	1787	1HB	GLN	231	4.514	7.397	32.171	1.00	0.00	H
ATOM	1788	2HB	GLN	231	6.080	6.653	31.699	1.00	0.00	H
ATOM	1789	1HG	GLN	231	4.974	4.914	30.554	1.00	0.00	H
ATOM	1790	2HG	GLN	231	3.369	5.699	30.840	1.00	0.00	H
ATOM	1791	1HE2	GLN	231	5.455	4.599	34.344	1.00	0.00	H
ATOM	1792	2HE2	GLN	231	6.259	5.479	33.017	1.00	0.00	H
ATOM	1793	N	ASP	232	2.981	8.885	30.475	1.00	0.00	N
ATOM	1794	CA	ASP	232	1.612	9.139	30.151	1.00	0.00	C
ATOM	1795	C	ASP	232	1.582	10.076	28.998	1.00	0.00	C
ATOM	1796	O	ASP	232	1.205	11.239	29.130	1.00	0.00	O
ATOM	1797	CB	ASP	232	0.813	9.726	31.322	1.00	0.00	C
ATOM	1798	CG	ASP	232	0.596	8.588	32.310	1.00	0.00	C
ATOM	1799	OD1	ASP	232	-0.379	7.816	32.104	1.00	0.00	O
ATOM	1800	OD2	ASP	232	1.392	8.476	33.280	1.00	0.00	O
ATOM	1801	H	ASP	232	3.425	9.372	31.265	1.00	0.00	H
ATOM	1802	HA	ASP	232	1.146	8.187	29.893	1.00	0.00	H
ATOM	1803	1HB	ASP	232	-0.123	10.094	30.903	1.00	0.00	H
ATOM	1804	2HB	ASP	232	1.422	10.527	31.741	1.00	0.00	H
ATOM	1805	N	LYS	233	1.911	9.483	27.834	1.00	0.00	N
ATOM	1806	CA	LYS	233	2.059	9.917	26.474	1.00	0.00	C
ATOM	1807	C	LYS	233	2.031	11.393	26.237	1.00	0.00	C
ATOM	1808	O	LYS	233	2.270	12.236	27.099	1.00	0.00	O
ATOM	1809	CB	LYS	233	0.968	9.331	25.555	1.00	0.00	C
ATOM	1810	CG	LYS	233	0.905	7.803	25.516	1.00	0.00	C
ATOM	1811	CD	LYS	233	-0.411	7.293	24.923	1.00	0.00	C
ATOM	1812	CE	LYS	233	-1.647	7.734	25.715	1.00	0.00	C
ATOM	1813	NZ	LYS	233	-2.871	7.215	25.066	1.00	0.00	N
ATOM	1814	H	LYS	233	2.102	8.477	27.947	1.00	0.00	H
ATOM	1815	HA	LYS	233	3.022	9.557	26.113	1.00	0.00	H
ATOM	1816	1HB	LYS	233	1.160	9.675	24.538	1.00	0.00	H
ATOM	1817	2HB	LYS	233	0.000	9.687	25.907	1.00	0.00	H
ATOM	1818	1HG	LYS	233	0.990	7.361	26.508	1.00	0.00	H
ATOM	1819	2HG	LYS	233	1.705	7.372	24.913	1.00	0.00	H
ATOM	1820	1HD	LYS	233	-0.472	6.205	24.876	1.00	0.00	H
ATOM	1821	2HD	LYS	233	-0.587	7.634	23.902	1.00	0.00	H
ATOM	1822	1HE	LYS	233	-1.695	8.822	25.749	1.00	0.00	H
ATOM	1823	2HE	LYS	233	-1.591	7.347	26.732	1.00	0.00	H
ATOM	1824	1HZ	LYS	233	-2.613	6.674	24.228	1.00	0.00	H
ATOM	1825	2HZ	LYS	233	-3.377	6.606	25.724	1.00	0.00	H
ATOM	1826	3HZ	LYS	233	-3.475	8.002	24.793	1.00	0.00	H
ATOM	1827	N	PHE	234	1.777	11.710	24.954	1.00	0.00	N
ATOM	1828	CA	PHE	234	1.759	13.034	24.418	1.00	0.00	C
ATOM	1829	C	PHE	234	0.709	13.786	25.149	1.00	0.00	C
ATOM	1830	O	PHE	234	0.895	14.969	25.441	1.00	0.00	O
ATOM	1831	CB	PHE	234	1.375	13.047	22.928	1.00	0.00	C

ATOM	1832	CG	PHE	234	2.317	12.149	22.193	1.00	0.00	C
ATOM	1833	CD1	PHE	234	3.608	12.540	21.919	1.00	0.00	C
ATOM	1834	CD2	PHE	234	1.899	10.909	21.762	1.00	0.00	C
ATOM	1835	CE1	PHE	234	4.466	11.707	21.239	1.00	0.00	C
ATOM	1836	CE2	PHE	234	2.752	10.072	21.081	1.00	0.00	C
ATOM	1837	CZ	PHE	234	4.040	10.469	20.818	1.00	0.00	C
ATOM	1838	H	PHE	234	1.579	10.934	24.305	1.00	0.00	H
ATOM	1839	HA	PHE	234	2.749	13.459	24.582	1.00	0.00	H
ATOM	1840	1HB	PHE	234	1.456	14.070	22.562	1.00	0.00	H
ATOM	1841	2HB	PHE	234	0.350	12.686	22.835	1.00	0.00	H
ATOM	1842	HD1	PHE	234	3.954	13.520	22.244	1.00	0.00	H
ATOM	1843	HD2	PHE	234	0.877	10.586	21.963	1.00	0.00	H
ATOM	1844	HE1	PHE	234	5.486	12.029	21.033	1.00	0.00	H
ATOM	1845	HE2	PHE	234	2.405	9.093	20.749	1.00	0.00	H
ATOM	1846	HZ	PHE	234	4.719	9.808	20.279	1.00	0.00	H
ATOM	1847	N	GLY	235	-0.428	13.104	25.425	1.00	0.00	N
ATOM	1848	CA	GLY	235	-1.482	13.680	26.208	1.00	0.00	C
ATOM	1849	C	GLY	235	-0.783	14.173	27.418	1.00	0.00	C
ATOM	1850	O	GLY	235	-0.341	13.387	28.255	1.00	0.00	O
ATOM	1851	H	GLY	235	-0.538	12.146	25.062	1.00	0.00	H
ATOM	1852	1HA	GLY	235	-2.238	12.934	26.454	1.00	0.00	H
ATOM	1853	2HA	GLY	235	-1.972	14.489	25.667	1.00	0.00	H
ATOM	1854	N	VAL	236	-0.631	15.508	27.495	1.00	0.00	N
ATOM	1855	CA	VAL	236	0.170	16.056	28.538	1.00	0.00	C
ATOM	1856	C	VAL	236	-0.596	16.087	29.799	1.00	0.00	C
ATOM	1857	O	VAL	236	-0.662	17.109	30.481	1.00	0.00	O
ATOM	1858	CB	VAL	236	0.648	17.440	28.268	1.00	0.00	C
ATOM	1859	CG1	VAL	236	1.634	17.359	27.103	1.00	0.00	C
ATOM	1860	CG2	VAL	236	-0.576	18.339	28.023	1.00	0.00	C
ATOM	1861	H	VAL	236	-1.087	16.125	26.808	1.00	0.00	H
ATOM	1862	HA	VAL	236	1.062	15.447	28.681	1.00	0.00	H
ATOM	1863	HB	VAL	236	1.129	17.798	29.177	1.00	0.00	H
ATOM	1864	1HG1	VAL	236	1.728	16.322	26.778	1.00	0.00	H
ATOM	1865	2HG1	VAL	236	1.269	17.967	26.275	1.00	0.00	H
ATOM	1866	3HG1	VAL	236	2.607	17.729	27.424	1.00	0.00	H
ATOM	1867	1HG2	VAL	236	-1.486	17.745	28.106	1.00	0.00	H
ATOM	1868	2HG2	VAL	236	-0.594	19.138	28.764	1.00	0.00	H
ATOM	1869	3HG2	VAL	236	-0.515	18.771	27.024	1.00	0.00	H
ATOM	1870	N	GLU	237	-1.195	14.948	30.156	1.00	0.00	N
ATOM	1871	CA	GLU	237	-1.760	14.911	31.454	1.00	0.00	C
ATOM	1872	C	GLU	237	-0.560	15.055	32.317	1.00	0.00	C
ATOM	1873	O	GLU	237	-0.590	15.716	33.347	1.00	0.00	O
ATOM	1874	CB	GLU	237	-2.441	13.574	31.794	1.00	0.00	C
ATOM	1875	CG	GLU	237	-3.838	13.423	31.190	1.00	0.00	C
ATOM	1876	CD	GLU	237	-4.819	14.039	32.179	1.00	0.00	C
ATOM	1877	OE1	GLU	237	-4.564	15.189	32.625	1.00	0.00	O
ATOM	1878	OE2	GLU	237	-5.825	13.359	32.515	1.00	0.00	O
ATOM	1879	H	GLU	237	-1.243	14.138	29.520	1.00	0.00	H
ATOM	1880	HA	GLU	237	-2.474	15.721	31.599	1.00	0.00	H
ATOM	1881	1HB	GLU	237	-2.579	13.411	32.862	1.00	0.00	H
ATOM	1882	2HB	GLU	237	-1.890	12.699	31.446	1.00	0.00	H
ATOM	1883	1HG	GLU	237	-4.013	12.355	31.056	1.00	0.00	H
ATOM	1884	2HG	GLU	237	-3.832	13.955	30.238	1.00	0.00	H
ATOM	1885	N	THR	238	0.559	14.451	31.880	1.00	0.00	N
ATOM	1886	CA	THR	238	1.759	14.474	32.658	1.00	0.00	C
ATOM	1887	C	THR	238	2.244	15.878	32.867	1.00	0.00	C
ATOM	1888	O	THR	238	2.386	16.320	34.006	1.00	0.00	O
ATOM	1889	CB	THR	238	2.848	13.716	31.974	1.00	0.00	C
ATOM	1890	OG1	THR	238	3.071	14.280	30.692	1.00	0.00	O
ATOM	1891	CG2	THR	238	2.418	12.248	31.829	1.00	0.00	C
ATOM	1892	H	THR	238	0.551	13.964	30.972	1.00	0.00	H
ATOM	1893	HA	THR	238	1.601	14.029	33.640	1.00	0.00	H
ATOM	1894	HB	THR	238	3.755	13.781	32.574	1.00	0.00	H
ATOM	1895	HG1	THR	238	3.511	15.205	30.795	1.00	0.00	H
ATOM	1896	1HG2	THR	238	1.425	12.115	32.259	1.00	0.00	H
ATOM	1897	2HG2	THR	238	2.394	11.978	30.773	1.00	0.00	H
ATOM	1898	3HG2	THR	238	3.128	11.607	32.351	1.00	0.00	H
ATOM	1899	N	LEU	239	2.493	16.631	31.778	1.00	0.00	N

ATOM	1900	CA	LEU	239	3.068	17.938	31.923	1.00	0.00	C
ATOM	1901	C	LEU	239	2.048	18.842	32.531	1.00	0.00	C
ATOM	1902	O	LEU	239	2.335	19.584	33.470	1.00	0.00	O
ATOM	1903	CB	LEU	239	3.477	18.540	30.565	1.00	0.00	C
ATOM	1904	CG	LEU	239	4.523	19.673	30.645	1.00	0.00	C
ATOM	1905	CD1	LEU	239	4.601	20.450	29.321	1.00	0.00	C
ATOM	1906	CD2	LEU	239	4.347	20.565	31.882	1.00	0.00	C
ATOM	1907	H	LEU	239	2.270	16.268	30.840	1.00	0.00	H
ATOM	1908	HA	LEU	239	3.941	17.863	32.570	1.00	0.00	H
ATOM	1909	1HB	LEU	239	2.584	18.951	30.093	1.00	0.00	H
ATOM	1910	2HB	LEU	239	3.903	17.743	29.955	1.00	0.00	H
ATOM	1911	HG	LEU	239	5.516	19.276	30.856	1.00	0.00	H
ATOM	1912	1HD1	LEU	239	3.893	20.026	28.608	1.00	0.00	H
ATOM	1913	2HD1	LEU	239	4.354	21.496	29.498	1.00	0.00	H
ATOM	1914	3HD1	LEU	239	5.610	20.378	28.916	1.00	0.00	H
ATOM	1915	1HD2	LEU	239	3.499	20.210	32.468	1.00	0.00	H
ATOM	1916	2HD2	LEU	239	5.250	20.526	32.490	1.00	0.00	H
ATOM	1917	3HD2	LEU	239	4.165	21.592	31.566	1.00	0.00	H
ATOM	1918	N	GLY	240	0.810	18.774	32.009	1.00	0.00	N
ATOM	1919	CA	GLY	240	-0.223	19.663	32.444	1.00	0.00	C
ATOM	1920	C	GLY	240	-0.528	19.425	33.885	1.00	0.00	C
ATOM	1921	O	GLY	240	-0.675	20.370	34.658	1.00	0.00	O
ATOM	1922	H	GLY	240	0.602	18.071	31.285	1.00	0.00	H
ATOM	1923	1HA	GLY	240	-1.127	19.497	31.859	1.00	0.00	H
ATOM	1924	2HA	GLY	240	0.096	20.697	32.316	1.00	0.00	H
ATOM	1925	N	GLU	241	-0.636	18.149	34.289	1.00	0.00	N
ATOM	1926	CA	GLU	241	-1.010	17.853	35.642	1.00	0.00	C
ATOM	1927	C	GLU	241	0.040	18.318	36.594	1.00	0.00	C
ATOM	1928	O	GLU	241	-0.278	18.862	37.650	1.00	0.00	O
ATOM	1929	CB	GLU	241	-1.230	16.361	35.924	1.00	0.00	C
ATOM	1930	CG	GLU	241	-1.628	16.065	37.370	1.00	0.00	C
ATOM	1931	CD	GLU	241	-1.804	14.559	37.469	1.00	0.00	C
ATOM	1932	OE1	GLU	241	-1.731	13.902	36.397	1.00	0.00	O
ATOM	1933	OE2	GLU	241	-2.014	14.044	38.601	1.00	0.00	O
ATOM	1934	H	GLU	241	-0.450	17.382	33.627	1.00	0.00	H
ATOM	1935	HA	GLU	241	-1.946	18.347	35.900	1.00	0.00	H
ATOM	1936	1HB	GLU	241	-0.347	15.748	35.741	1.00	0.00	H
ATOM	1937	2HB	GLU	241	-2.016	15.914	35.315	1.00	0.00	H
ATOM	1938	1HG	GLU	241	-2.558	16.602	37.550	1.00	0.00	H
ATOM	1939	2HG	GLU	241	-0.812	16.427	37.995	1.00	0.00	H
ATOM	1940	N	SER	242	1.327	18.111	36.263	1.00	0.00	N
ATOM	1941	CA	SER	242	2.331	18.491	37.212	1.00	0.00	C
ATOM	1942	C	SER	242	2.290	19.972	37.418	1.00	0.00	C
ATOM	1943	O	SER	242	2.237	20.450	38.551	1.00	0.00	O
ATOM	1944	CB	SER	242	3.752	18.117	36.756	1.00	0.00	C
ATOM	1945	OG	SER	242	3.879	16.704	36.680	1.00	0.00	O
ATOM	1946	H	SER	242	1.582	17.693	35.357	1.00	0.00	H
ATOM	1947	HA	SER	242	2.144	17.988	38.161	1.00	0.00	H
ATOM	1948	1HB	SER	242	4.483	18.502	37.466	1.00	0.00	H
ATOM	1949	2HB	SER	242	3.951	18.545	35.773	1.00	0.00	H
ATOM	1950	HG	SER	242	2.944	16.278	36.604	1.00	0.00	H
ATOM	1951	N	VAL	243	2.292	20.747	36.317	1.00	0.00	N
ATOM	1952	CA	VAL	243	2.308	22.172	36.473	1.00	0.00	C
ATOM	1953	C	VAL	243	1.029	22.598	37.118	1.00	0.00	C
ATOM	1954	O	VAL	243	1.021	23.439	38.016	1.00	0.00	O
ATOM	1955	CB	VAL	243	2.446	22.904	35.165	1.00	0.00	C
ATOM	1956	CG1	VAL	243	2.403	24.420	35.439	1.00	0.00	C
ATOM	1957	CG2	VAL	243	3.745	22.442	34.483	1.00	0.00	C
ATOM	1958	H	VAL	243	2.282	20.323	35.378	1.00	0.00	H
ATOM	1959	HA	VAL	243	3.156	22.445	37.100	1.00	0.00	H
ATOM	1960	HB	VAL	243	1.620	22.615	34.513	1.00	0.00	H
ATOM	1961	1HG1	VAL	243	2.283	24.593	36.508	1.00	0.00	H
ATOM	1962	2HG1	VAL	243	3.331	24.877	35.098	1.00	0.00	H
ATOM	1963	3HG1	VAL	243	1.563	24.862	34.903	1.00	0.00	H
ATOM	1964	1HG2	VAL	243	4.242	21.702	35.110	1.00	0.00	H
ATOM	1965	2HG2	VAL	243	3.510	21.997	33.516	1.00	0.00	H
ATOM	1966	3HG2	VAL	243	4.404	23.297	34.338	1.00	0.00	H
ATOM	1967	N	ALA	244	-0.089	21.991	36.686	1.00	0.00	N

ATOM	1968	CA	ALA	244	-1.381	22.364	37.178	1.00	0.00	C
ATOM	1969	C	ALA	244	-1.464	22.089	38.641	1.00	0.00	C
ATOM	1970	O	ALA	244	-1.979	22.906	39.397	1.00	0.00	O
ATOM	1971	CB	ALA	244	-2.522	21.587	36.498	1.00	0.00	C
ATOM	1972	H	ALA	244	-0.015	21.240	35.984	1.00	0.00	H
ATOM	1973	HA	ALA	244	-1.550	23.426	37.004	1.00	0.00	H
ATOM	1974	1HB	ALA	244	-2.105	20.896	35.764	1.00	0.00	H
ATOM	1975	2HB	ALA	244	-3.078	21.026	37.249	1.00	0.00	H
ATOM	1976	3HB	ALA	244	-3.191	22.287	35.997	1.00	0.00	H
ATOM	1977	N	GLN	245	-0.932	20.945	39.095	1.00	0.00	N
ATOM	1978	CA	GLN	245	-1.081	20.586	40.472	1.00	0.00	C
ATOM	1979	C	GLN	245	-0.434	21.623	41.326	1.00	0.00	C
ATOM	1980	O	GLN	245	-0.974	22.004	42.364	1.00	0.00	O
ATOM	1981	CB	GLN	245	-0.444	19.224	40.788	1.00	0.00	C
ATOM	1982	CG	GLN	245	-0.680	18.744	42.219	1.00	0.00	C
ATOM	1983	CD	GLN	245	-0.143	17.325	42.312	1.00	0.00	C
ATOM	1984	OE1	GLN	245	0.422	16.805	41.351	1.00	0.00	O
ATOM	1985	NE2	GLN	245	-0.323	16.683	43.496	1.00	0.00	N
ATOM	1986	H	GLN	245	-0.416	20.325	38.453	1.00	0.00	H
ATOM	1987	HA	GLN	245	-2.141	20.521	40.715	1.00	0.00	H
ATOM	1988	1HB	GLN	245	0.632	19.305	40.637	1.00	0.00	H
ATOM	1989	2HB	GLN	245	-0.869	18.481	40.113	1.00	0.00	H
ATOM	1990	1HG	GLN	245	-1.754	18.779	42.398	1.00	0.00	H
ATOM	1991	2HG	GLN	245	-0.140	19.422	42.880	1.00	0.00	H
ATOM	1992	1HE2	GLN	245	0.020	15.719	43.616	1.00	0.00	H
ATOM	1993	2HE2	GLN	245	-0.802	17.160	44.272	1.00	0.00	H
ATOM	1994	N	LEU	246	0.738	22.131	40.904	1.00	0.00	N
ATOM	1995	CA	LEU	246	1.420	23.068	41.744	1.00	0.00	C
ATOM	1996	C	LEU	246	0.544	24.255	41.995	1.00	0.00	C
ATOM	1997	O	LEU	246	0.235	24.566	43.143	1.00	0.00	O
ATOM	1998	CB	LEU	246	2.728	23.589	41.122	1.00	0.00	C
ATOM	1999	CG	LEU	246	3.804	22.505	40.924	1.00	0.00	C
ATOM	2000	CD1	LEU	246	5.081	23.092	40.304	1.00	0.00	C
ATOM	2001	CD2	LEU	246	4.072	21.740	42.227	1.00	0.00	C
ATOM	2002	H	LEU	246	1.136	21.851	39.996	1.00	0.00	H
ATOM	2003	HA	LEU	246	1.667	22.598	42.696	1.00	0.00	H
ATOM	2004	1HB	LEU	246	3.141	24.351	41.781	1.00	0.00	H
ATOM	2005	2HB	LEU	246	2.498	24.012	40.144	1.00	0.00	H
ATOM	2006	HG	LEU	246	3.451	21.712	40.263	1.00	0.00	H
ATOM	2007	1HD1	LEU	246	4.946	24.160	40.137	1.00	0.00	H
ATOM	2008	2HD1	LEU	246	5.920	22.933	40.981	1.00	0.00	H
ATOM	2009	3HD1	LEU	246	5.283	22.598	39.353	1.00	0.00	H
ATOM	2010	1HD2	LEU	246	3.435	22.135	43.018	1.00	0.00	H
ATOM	2011	2HD2	LEU	246	3.853	20.682	42.079	1.00	0.00	H
ATOM	2012	3HD2	LEU	246	5.117	21.858	42.510	1.00	0.00	H
ATOM	2013	N	GLN	247	0.093	24.944	40.933	1.00	0.00	N
ATOM	2014	CA	GLN	247	-0.684	26.129	41.168	1.00	0.00	C
ATOM	2015	C	GLN	247	-2.052	25.791	41.680	1.00	0.00	C
ATOM	2016	O	GLN	247	-2.532	26.370	42.654	1.00	0.00	O
ATOM	2017	CB	GLN	247	-0.881	26.986	39.907	1.00	0.00	C
ATOM	2018	CG	GLN	247	-1.694	26.296	38.811	1.00	0.00	C
ATOM	2019	CD	GLN	247	-1.848	27.279	37.660	1.00	0.00	C
ATOM	2020	OE1	GLN	247	-2.517	26.995	36.668	1.00	0.00	O
ATOM	2021	NE2	GLN	247	-1.214	28.474	37.797	1.00	0.00	N
ATOM	2022	H	GLN	247	0.299	24.630	39.974	1.00	0.00	H
ATOM	2023	HA	GLN	247	-0.207	26.775	41.904	1.00	0.00	H
ATOM	2024	1HB	GLN	247	0.100	27.223	39.495	1.00	0.00	H
ATOM	2025	2HB	GLN	247	-1.407	27.897	40.189	1.00	0.00	H
ATOM	2026	1HG	GLN	247	-2.662	26.030	39.233	1.00	0.00	H
ATOM	2027	2HG	GLN	247	-1.144	25.408	38.499	1.00	0.00	H
ATOM	2028	1HE2	GLN	247	-1.284	29.182	37.052	1.00	0.00	H
ATOM	2029	2HE2	GLN	247	-0.663	28.670	38.645	1.00	0.00	H
ATOM	2030	N	ALA	248	-2.695	24.812	41.023	1.00	0.00	N
ATOM	2031	CA	ALA	248	-4.067	24.432	41.207	1.00	0.00	C
ATOM	2032	C	ALA	248	-4.356	23.822	42.539	1.00	0.00	C
ATOM	2033	O	ALA	248	-5.467	24.009	43.033	1.00	0.00	O
ATOM	2034	CB	ALA	248	-4.564	23.434	40.146	1.00	0.00	C
ATOM	2035	H	ALA	248	-2.153	24.285	40.322	1.00	0.00	H

```
ATOM   2036  HA  ALA   248      -4.686  25.323  41.108  1.00  0.00           H
ATOM   2037 1HB  ALA   248      -3.755  23.209  39.450  1.00  0.00           H
ATOM   2038 2HB  ALA   248      -4.887  22.514  40.634  1.00  0.00           H
ATOM   2039 3HB  ALA   248      -5.401  23.869  39.600  1.00  0.00           H
ATOM   2040  N   TRP   249      -3.392  23.071  43.125  1.00  0.00           N
ATOM   2041  CA  TRP   249      -3.588  22.300  44.332  1.00  0.00           C
ATOM   2042  C   TRP   249      -4.401  23.052  45.341  1.00  0.00           C
ATOM   2043  O   TRP   249      -4.442  24.282  45.333  1.00  0.00           O
ATOM   2044  CB  TRP   249      -2.297  21.836  45.028  1.00  0.00           C
ATOM   2045  CG  TRP   249      -2.564  20.972  46.241  1.00  0.00           C
ATOM   2046  CD1 TRP   249      -2.739  21.331  47.546  1.00  0.00           C
ATOM   2047  CD2 TRP   249      -2.704  19.543  46.192  1.00  0.00           C
ATOM   2048  NE1 TRP   249      -2.978  20.216  48.314  1.00  0.00           N
ATOM   2049  CE2 TRP   249      -2.959  19.109  47.493  1.00  0.00           C
ATOM   2050  CE3 TRP   249      -2.628  18.666  45.150  1.00  0.00           C
ATOM   2051  CZ2 TRP   249      -3.143  17.783  47.771  1.00  0.00           C
ATOM   2052  CZ3 TRP   249      -2.812  17.330  45.433  1.00  0.00           C
ATOM   2053  CH2 TRP   249      -3.064  16.898  46.718  1.00  0.00           C
ATOM   2054  H   TRP   249      -2.462  23.048  42.682  1.00  0.00           H
ATOM   2055  HA  TRP   249      -4.108  21.363  44.130  1.00  0.00           H
ATOM   2056 1HB  TRP   249      -1.685  22.666  45.379  1.00  0.00           H
ATOM   2057 2HB  TRP   249      -1.654  21.245  44.374  1.00  0.00           H
ATOM   2058  HD1 TRP   249      -2.695  22.352  47.924  1.00  0.00           H
ATOM   2059  HE1 TRP   249      -3.143  20.209  49.330  1.00  0.00           H
ATOM   2060  HE3 TRP   249      -2.429  19.008  44.134  1.00  0.00           H
ATOM   2061  HZ2 TRP   249      -3.344  17.439  48.785  1.00  0.00           H
ATOM   2062  HZ3 TRP   249      -2.757  16.600  44.625  1.00  0.00           H
ATOM   2063  HH2 TRP   249      -3.203  15.833  46.904  1.00  0.00           H
ATOM   2064  N   TRP   250      -5.066  22.282  46.230  1.00  0.00           N
ATOM   2065  CA  TRP   250      -5.997  22.750  47.219  1.00  0.00           C
ATOM   2066  C   TRP   250      -5.505  24.012  47.835  1.00  0.00           C
ATOM   2067  O   TRP   250      -4.711  24.006  48.775  1.00  0.00           O
ATOM   2068  CB  TRP   250      -6.252  21.725  48.339  1.00  0.00           C
ATOM   2069  CG  TRP   250      -7.228  22.179  49.396  1.00  0.00           C
ATOM   2070  CD1 TRP   250      -7.802  23.402  49.587  1.00  0.00           C
ATOM   2071  CD2 TRP   250      -7.744  21.323  50.426  1.00  0.00           C
ATOM   2072  NE1 TRP   250      -8.646  23.361  50.672  1.00  0.00           N
ATOM   2073  CE2 TRP   250      -8.620  22.086  51.197  1.00  0.00           C
ATOM   2074  CE3 TRP   250      -7.510  20.007  50.703  1.00  0.00           C
ATOM   2075  CZ2 TRP   250      -9.280  21.540  52.262  1.00  0.00           C
ATOM   2076  CZ3 TRP   250      -8.174  19.460  51.779  1.00  0.00           C
ATOM   2077  CH2 TRP   250      -9.043  20.212  52.543  1.00  0.00           C
ATOM   2078  H   TRP   250      -4.889  21.267  46.195  1.00  0.00           H
ATOM   2079  HA  TRP   250      -6.968  22.940  46.763  1.00  0.00           H
ATOM   2080 1HB  TRP   250      -5.303  21.518  48.834  1.00  0.00           H
ATOM   2081 2HB  TRP   250      -6.655  20.819  47.886  1.00  0.00           H
ATOM   2082  HD1 TRP   250      -7.618  24.281  48.970  1.00  0.00           H
ATOM   2083  HE1 TRP   250      -9.203  24.149  51.031  1.00  0.00           H
ATOM   2084  HE3 TRP   250      -6.825  19.413  50.097  1.00  0.00           H
ATOM   2085  HZ2 TRP   250      -9.967  22.132  52.865  1.00  0.00           H
ATOM   2086  HZ3 TRP   250      -8.009  18.412  52.031  1.00  0.00           H
ATOM   2087  HH2 TRP   250      -9.552  19.745  53.386  1.00  0.00           H
ATOM   2088  N   TYR   251      -5.973  25.140  47.277  1.00  0.00           N
ATOM   2089  CA  TYR   251      -5.632  26.446  47.746  1.00  0.00           C
ATOM   2090  C   TYR   251      -6.001  27.329  46.598  1.00  0.00           C
ATOM   2091  O   TYR   251      -6.391  26.827  45.546  1.00  0.00           O
ATOM   2092  CB  TYR   251      -4.122  26.588  48.038  1.00  0.00           C
ATOM   2093  CG  TYR   251      -3.855  27.870  48.753  1.00  0.00           C
ATOM   2094  CD1 TYR   251      -4.004  27.935  50.120  1.00  0.00           C
ATOM   2095  CD2 TYR   251      -3.457  29.002  48.078  1.00  0.00           C
ATOM   2096  CE1 TYR   251      -3.762  29.104  50.802  1.00  0.00           C
ATOM   2097  CE2 TYR   251      -3.213  30.175  48.753  1.00  0.00           C
ATOM   2098  CZ  TYR   251      -3.365  30.227  50.118  1.00  0.00           C
ATOM   2099  OH  TYR   251      -3.116  31.430  50.814  1.00  0.00           O
ATOM   2100  H   TYR   251      -6.609  25.060  46.471  1.00  0.00           H
ATOM   2101  HA  TYR   251      -6.191  26.697  48.646  1.00  0.00           H
ATOM   2102 1HB  TYR   251      -3.557  26.581  47.105  1.00  0.00           H
ATOM   2103 2HB  TYR   251      -3.780  25.761  48.660  1.00  0.00           H
```

```
ATOM   2104  HD1 TYR   251      -4.318  27.047  50.669  1.00  0.00           H
ATOM   2105  HD2 TYR   251      -3.333  28.968  46.995  1.00  0.00           H
ATOM   2106  HE1 TYR   251      -3.885  29.139  51.884  1.00  0.00           H
ATOM   2107  HE2 TYR   251      -2.899  31.063  48.205  1.00  0.00           H
ATOM   2108  HH  TYR   251      -2.228  31.838  50.488  1.00  0.00           H
ATOM   2109  N   LYS   252      -5.927  28.662  46.765  1.00  0.00           N
ATOM   2110  CA  LYS   252      -6.222  29.485  45.633  1.00  0.00           C
ATOM   2111  C   LYS   252      -5.202  29.112  44.610  1.00  0.00           C
ATOM   2112  O   LYS   252      -5.524  28.799  43.465  1.00  0.00           O
ATOM   2113  CB  LYS   252      -6.079  30.989  45.931  1.00  0.00           C
ATOM   2114  CG  LYS   252      -7.160  31.532  46.869  1.00  0.00           C
ATOM   2115  CD  LYS   252      -7.078  30.987  48.297  1.00  0.00           C
ATOM   2116  CE  LYS   252      -6.052  31.707  49.174  1.00  0.00           C
ATOM   2117  NZ  LYS   252      -6.089  31.160  50.549  1.00  0.00           N
ATOM   2118  H   LYS   252      -5.668  29.073  47.672  1.00  0.00           H
ATOM   2119  HA  LYS   252      -7.240  29.219  45.350  1.00  0.00           H
ATOM   2120 1HB  LYS   252      -6.133  31.616  45.041  1.00  0.00           H
ATOM   2121 2HB  LYS   252      -5.133  31.250  46.405  1.00  0.00           H
ATOM   2122 1HG  LYS   252      -8.134  31.258  46.464  1.00  0.00           H
ATOM   2123 2HG  LYS   252      -7.057  32.615  46.920  1.00  0.00           H
ATOM   2124 1HD  LYS   252      -6.801  29.934  48.350  1.00  0.00           H
ATOM   2125 2HD  LYS   252      -8.015  31.057  48.848  1.00  0.00           H
ATOM   2126 1HE  LYS   252      -6.276  32.773  49.211  1.00  0.00           H
ATOM   2127 2HE  LYS   252      -5.050  31.569  48.765  1.00  0.00           H
ATOM   2128 1HZ  LYS   252      -6.799  30.416  50.604  1.00  0.00           H
ATOM   2129 2HZ  LYS   252      -5.166  30.771  50.789  1.00  0.00           H
ATOM   2130 3HZ  LYS   252      -6.327  31.911  51.211  1.00  0.00           H
ATOM   2131  N   ALA   253      -3.928  29.121  45.036  1.00  0.00           N
ATOM   2132  CA  ALA   253      -2.828  28.699  44.224  1.00  0.00           C
ATOM   2133  C   ALA   253      -1.768  28.363  45.213  1.00  0.00           C
ATOM   2134  O   ALA   253      -1.332  29.233  45.965  1.00  0.00           O
ATOM   2135  CB  ALA   253      -2.270  29.807  43.315  1.00  0.00           C
ATOM   2136  H   ALA   253      -3.733  29.447  45.993  1.00  0.00           H
ATOM   2137  HA  ALA   253      -3.100  27.835  43.617  1.00  0.00           H
ATOM   2138 1HB  ALA   253      -2.837  30.724  43.470  1.00  0.00           H
ATOM   2139 2HB  ALA   253      -1.221  29.982  43.557  1.00  0.00           H
ATOM   2140 3HB  ALA   253      -2.355  29.499  42.272  1.00  0.00           H
ATOM   2141  N   ASP   254      -1.325  27.092  45.273  1.00  0.00           N
ATOM   2142  CA  ASP   254      -0.364  26.857  46.306  1.00  0.00           C
ATOM   2143  C   ASP   254       0.945  26.444  45.725  1.00  0.00           C
ATOM   2144  O   ASP   254       1.185  25.290  45.380  1.00  0.00           O
ATOM   2145  CB  ASP   254      -0.826  25.827  47.354  1.00  0.00           C
ATOM   2146  CG  ASP   254      -1.081  24.488  46.688  1.00  0.00           C
ATOM   2147  OD1 ASP   254      -1.331  24.467  45.453  1.00  0.00           O
ATOM   2148  OD2 ASP   254      -1.024  23.463  47.416  1.00  0.00           O
ATOM   2149  H   ASP   254      -1.649  26.354  44.631  1.00  0.00           H
ATOM   2150  HA  ASP   254      -0.204  27.758  46.897  1.00  0.00           H
ATOM   2151 1HB  ASP   254      -1.746  26.166  47.829  1.00  0.00           H
ATOM   2152 2HB  ASP   254      -0.058  25.702  48.117  1.00  0.00           H
ATOM   2153  N   PRO   255       1.799  27.413  45.598  1.00  0.00           N
ATOM   2154  CA  PRO   255       3.131  27.150  45.144  1.00  0.00           C
ATOM   2155  C   PRO   255       3.913  26.561  46.271  1.00  0.00           C
ATOM   2156  O   PRO   255       5.002  26.041  46.034  1.00  0.00           O
ATOM   2157  CB  PRO   255       3.682  28.485  44.632  1.00  0.00           C
ATOM   2158  CG  PRO   255       2.680  29.543  45.131  1.00  0.00           C
ATOM   2159  CD  PRO   255       1.368  28.760  45.269  1.00  0.00           C
ATOM   2160  HA  PRO   255       3.084  26.448  44.310  1.00  0.00           H
ATOM   2161 1HB  PRO   255       3.704  28.380  43.547  1.00  0.00           H
ATOM   2162 2HB  PRO   255       4.670  28.570  45.083  1.00  0.00           H
ATOM   2163 1HG  PRO   255       2.587  30.360  44.416  1.00  0.00           H
ATOM   2164 2HG  PRO   255       2.999  29.964  46.083  1.00  0.00           H
ATOM   2165 1HD  PRO   255       0.737  29.170  46.057  1.00  0.00           H
ATOM   2166 2HD  PRO   255       0.795  28.769  44.341  1.00  0.00           H
ATOM   2167  N   ASN   256       3.382  26.645  47.505  1.00  0.00           N
ATOM   2168  CA  ASN   256       4.103  26.175  48.650  1.00  0.00           C
ATOM   2169  C   ASN   256       4.282  24.693  48.576  1.00  0.00           C
ATOM   2170  O   ASN   256       5.364  24.186  48.865  1.00  0.00           O
ATOM   2171  CB  ASN   256       3.409  26.489  49.988  1.00  0.00           C
```

```
ATOM   2172  CG  ASN   256       2.086  25.743  50.031  1.00  0.00           C
ATOM   2173  OD1 ASN   256       1.248  25.897  49.145  1.00  0.00           O
ATOM   2174  ND2 ASN   256       1.893  24.904  51.084  1.00  0.00           N
ATOM   2175  H   ASN   256       2.444  27.052  47.627  1.00  0.00           H
ATOM   2176  HA  ASN   256       5.086  26.643  48.695  1.00  0.00           H
ATOM   2177 1HB  ASN   256       3.241  27.564  50.046  1.00  0.00           H
ATOM   2178 2HB  ASN   256       4.058  26.160  50.799  1.00  0.00           H
ATOM   2179 1HD2 ASN   256       1.017  24.367  51.161  1.00  0.00           H
ATOM   2180 2HD2 ASN   256       2.622  24.805  51.804  1.00  0.00           H
ATOM   2181  N   ASP   257       3.235  23.948  48.173  1.00  0.00           N
ATOM   2182  CA  ASP   257       3.373  22.521  48.199  1.00  0.00           C
ATOM   2183  C   ASP   257       4.172  22.062  47.023  1.00  0.00           C
ATOM   2184  O   ASP   257       4.248  22.734  45.995  1.00  0.00           O
ATOM   2185  CB  ASP   257       2.036  21.752  48.210  1.00  0.00           C
ATOM   2186  CG  ASP   257       1.274  22.042  46.925  1.00  0.00           C
ATOM   2187  OD1 ASP   257       1.721  22.934  46.156  1.00  0.00           O
ATOM   2188  OD2 ASP   257       0.230  21.375  46.697  1.00  0.00           O
ATOM   2189  H   ASP   257       2.360  24.390  47.855  1.00  0.00           H
ATOM   2190  HA  ASP   257       3.880  22.211  49.112  1.00  0.00           H
ATOM   2191 1HB  ASP   257       1.440  22.071  49.065  1.00  0.00           H
ATOM   2192 2HB  ASP   257       2.233  20.682  48.282  1.00  0.00           H
ATOM   2193  N   PHE   258       4.823  20.892  47.190  1.00  0.00           N
ATOM   2194  CA  PHE   258       5.592  20.266  46.156  1.00  0.00           C
ATOM   2195  C   PHE   258       4.993  18.915  45.937  1.00  0.00           C
ATOM   2196  O   PHE   258       4.476  18.303  46.870  1.00  0.00           O
ATOM   2197  CB  PHE   258       7.071  20.059  46.515  1.00  0.00           C
ATOM   2198  CG  PHE   258       7.636  19.177  45.458  1.00  0.00           C
ATOM   2199  CD1 PHE   258       7.941  19.671  44.211  1.00  0.00           C
ATOM   2200  CD2 PHE   258       7.855  17.846  45.722  1.00  0.00           C
ATOM   2201  CE1 PHE   258       8.460  18.842  43.243  1.00  0.00           C
ATOM   2202  CE2 PHE   258       8.375  17.016  44.760  1.00  0.00           C
ATOM   2203  CZ  PHE   258       8.679  17.514  43.517  1.00  0.00           C
ATOM   2204  H   PHE   258       4.764  20.425  48.106  1.00  0.00           H
ATOM   2205  HA  PHE   258       5.505  20.902  45.275  1.00  0.00           H
ATOM   2206 1HB  PHE   258       7.082  19.591  47.499  1.00  0.00           H
ATOM   2207 2HB  PHE   258       7.525  21.049  46.518  1.00  0.00           H
ATOM   2208  HD1 PHE   258       7.770  20.724  43.988  1.00  0.00           H
ATOM   2209  HD2 PHE   258       7.613  17.445  46.706  1.00  0.00           H
ATOM   2210  HE1 PHE   258       8.697  19.240  42.256  1.00  0.00           H
ATOM   2211  HE2 PHE   258       8.546  15.962  44.982  1.00  0.00           H
ATOM   2212  HZ  PHE   258       9.092  16.858  42.750  1.00  0.00           H
ATOM   2213  N   THR   259       5.027  18.416  44.685  1.00  0.00           N
ATOM   2214  CA  THR   259       4.421  17.142  44.438  1.00  0.00           C
ATOM   2215  C   THR   259       5.332  16.310  43.599  1.00  0.00           C
ATOM   2216  O   THR   259       6.119  16.829  42.810  1.00  0.00           O
ATOM   2217  CB  THR   259       3.119  17.232  43.697  1.00  0.00           C
ATOM   2218  OG1 THR   259       2.494  15.958  43.645  1.00  0.00           O
ATOM   2219  CG2 THR   259       3.392  17.757  42.279  1.00  0.00           C
ATOM   2220  H   THR   259       5.479  18.939  43.922  1.00  0.00           H
ATOM   2221  HA  THR   259       4.238  16.635  45.385  1.00  0.00           H
ATOM   2222  HB  THR   259       2.458  17.915  44.229  1.00  0.00           H
ATOM   2223  HG1 THR   259       1.471  16.077  43.610  1.00  0.00           H
ATOM   2224 1HG2 THR   259       4.460  17.935  42.156  1.00  0.00           H
ATOM   2225 2HG2 THR   259       3.061  17.019  41.547  1.00  0.00           H
ATOM   2226 3HG2 THR   259       2.848  18.689  42.125  1.00  0.00           H
ATOM   2227  N   TYR   260       5.261  14.975  43.780  1.00  0.00           N
ATOM   2228  CA  TYR   260       6.022  14.083  42.957  1.00  0.00           C
ATOM   2229  C   TYR   260       5.075  13.034  42.471  1.00  0.00           C
ATOM   2230  O   TYR   260       4.032  12.797  43.079  1.00  0.00           O
ATOM   2231  CB  TYR   260       7.210  13.401  43.665  1.00  0.00           C
ATOM   2232  CG  TYR   260       6.732  12.520  44.769  1.00  0.00           C
ATOM   2233  CD1 TYR   260       6.376  13.049  45.988  1.00  0.00           C
ATOM   2234  CD2 TYR   260       6.661  11:158  44.588  1.00  0.00           C
ATOM   2235  CE1 TYR   260       5.945  12.233  47.007  1.00  0.00           C
ATOM   2236  CE2 TYR   260       6.231  10.336  45.603  1.00  0.00           C
ATOM   2237  CZ  TYR   260       5.872  10.874  46.815  1.00  0.00           C
ATOM   2238  OH  TYR   260       5.431  10.033  47.859  1.00  0.00           O
ATOM   2239  H   TYR   260       4.652  14.592  44.518  1.00  0.00           H
```

ATOM	2240	HA	TYR	260	6.427	14.679	42.139	1.00	0.00	H
ATOM	2241	1HB	TYR	260	7.884	14.144	44.091	1.00	0.00	H
ATOM	2242	2HB	TYR	260	7.778	12.789	42.963	1.00	0.00	H
ATOM	2243	HD1	TYR	260	6.436	14.125	46.147	1.00	0.00	H
ATOM	2244	HD2	TYR	260	6.948	10.725	43.629	1.00	0.00	H
ATOM	2245	HE1	TYR	260	5.661	12.663	47.967	1.00	0.00	H
ATOM	2246	HE2	TYR	260	6.175	9.258	45.446	1.00	0.00	H
ATOM	2247	HH	TYR	260	4.745	10.536	48.439	1.00	0.00	H
ATOM	2248	N	GLU	261	5.408	12.390	41.336	1.00	0.00	N
ATOM	2249	CA	GLU	261	4.521	11.412	40.775	1.00	0.00	C
ATOM	2250	C	GLU	261	5.158	10.065	40.886	1.00	0.00	C
ATOM	2251	O	GLU	261	6.286	9.925	41.356	1.00	0.00	O
ATOM	2252	CB	GLU	261	4.219	11.655	39.286	1.00	0.00	C
ATOM	2253	CG	GLU	261	3.389	12.917	39.035	1.00	0.00	C
ATOM	2254	CD	GLU	261	4.257	14.127	39.348	1.00	0.00	C
ATOM	2255	OE1	GLU	261	5.409	14.181	38.841	1.00	0.00	O
ATOM	2256	OE2	GLU	261	3.779	15.013	40.106	1.00	0.00	O
ATOM	2257	H	GLU	261	6.301	12.600	40.869	1.00	0.00	H
ATOM	2258	HA	GLU	261	3.582	11.430	41.329	1.00	0.00	H
ATOM	2259	1HB	GLU	261	3.659	10.843	38.821	1.00	0.00	H
ATOM	2260	2HB	GLU	261	5.116	11.772	38.678	1.00	0.00	H
ATOM	2261	1HG	GLU	261	2.518	12.887	39.689	1.00	0.00	H
ATOM	2262	2HG	GLU	261	3.084	12.921	37.988	1.00	0.00	H
ATOM	2263	N	ARG	262	4.409	9.024	40.474	1.00	0.00	N
ATOM	2264	CA	ARG	262	4.912	7.682	40.478	1.00	0.00	C
ATOM	2265	C	ARG	262	5.836	7.571	39.313	1.00	0.00	C
ATOM	2266	O	ARG	262	5.746	8.344	38.359	1.00	0.00	O
ATOM	2267	CB	ARG	262	3.821	6.611	40.302	1.00	0.00	C
ATOM	2268	CG	ARG	262	2.842	6.530	41.475	1.00	0.00	C
ATOM	2269	CD	ARG	262	1.728	5.502	41.266	1.00	0.00	C
ATOM	2270	NE	ARG	262	0.894	5.979	40.127	1.00	0.00	N
ATOM	2271	CZ	ARG	262	-0.207	5.271	39.738	1.00	0.00	C
ATOM	2272	NH1	ARG	262	-0.549	4.125	40.395	1.00	0.00	N
ATOM	2273	NH2	ARG	262	-0.967	5.711	38.692	1.00	0.00	N
ATOM	2274	H	ARG	262	3.447	9.197	40.146	1.00	0.00	H
ATOM	2275	HA	ARG	262	5.428	7.546	41.428	1.00	0.00	H
ATOM	2276	1HB	ARG	262	4.212	5.599	40.193	1.00	0.00	H
ATOM	2277	2HB	ARG	262	3.193	6.763	39.423	1.00	0.00	H
ATOM	2278	1HG	ARG	262	2.330	7.471	41.677	1.00	0.00	H
ATOM	2279	2HG	ARG	262	3.316	6.252	42.416	1.00	0.00	H
ATOM	2280	1HD	ARG	262	1.153	5.454	42.191	1.00	0.00	H
ATOM	2281	2HD	ARG	262	2.205	4.548	41.041	1.00	0.00	H
ATOM	2282	HE	ARG	262	1.148	6.845	39.631	1.00	0.00	H
ATOM	2283	1HH1	ARG	262	0.023	3.793	41.184	1.00	0.00	H
ATOM	2284	2HH1	ARG	262	-1.379	3.591	40.101	1.00	0.00	H
ATOM	2285	1HH2	ARG	262	-0.709	6.576	38.196	1.00	0.00	H
ATOM	2286	2HH2	ARG	262	-1.797	5.177	38.398	1.00	0.00	H
ATOM	2287	N	ARG	263	6.773	6.608	39.364	1.00	0.00	N
ATOM	2288	CA	ARG	263	7.701	6.525	38.280	1.00	0.00	C
ATOM	2289	C	ARG	263	8.128	5.105	38.141	1.00	0.00	C
ATOM	2290	O	ARG	263	8.055	4.322	39.086	1.00	0.00	O
ATOM	2291	CB	ARG	263	8.985	7.313	38.573	1.00	0.00	C
ATOM	2292	CG	ARG	263	8.733	8.781	38.921	1.00	0.00	C
ATOM	2293	CD	ARG	263	9.924	9.441	39.615	1.00	0.00	C
ATOM	2294	NE	ARG	263	10.023	8.832	40.972	1.00	0.00	N
ATOM	2295	CZ	ARG	263	9.671	9.547	42.081	1.00	0.00	C
ATOM	2296	NH1	ARG	263	9.233	10.835	41.951	1.00	0.00	N
ATOM	2297	NH2	ARG	263	9.768	8.978	43.318	1.00	0.00	N
ATOM	2298	H	ARG	263	6.820	5.952	40.157	1.00	0.00	H
ATOM	2299	HA	ARG	263	7.198	6.866	37.375	1.00	0.00	H
ATOM	2300	1HB	ARG	263	9.682	7.333	37.735	1.00	0.00	H
ATOM	2301	2HB	ARG	263	9.557	6.915	39.411	1.00	0.00	H
ATOM	2302	1HG	ARG	263	7.884	8.918	39.591	1.00	0.00	H
ATOM	2303	2HG	ARG	263	8.522	9.394	38.045	1.00	0.00	H
ATOM	2304	1HD	ARG	263	9.709	10.508	39.660	1.00	0.00	H
ATOM	2305	2HD	ARG	263	10.801	9.226	39.005	1.00	0.00	H
ATOM	2306	HE	ARG	263	10.359	7.863	41.074	1.00	0.00	H
ATOM	2307	1HH1	ARG	263	9.168	11.265	41.017	1.00	0.00	H

ATOM	2308	2HH1	ARG	263	8.967	11.375	42.786	1.00	0.00	H
ATOM	2309	1HH2	ARG	263	10.106	8.010	43.414	1.00	0.00	H
ATOM	2310	2HH2	ARG	263	9.502	9.516	44.154	1.00	-0.00	H
ATOM	2311	N	LYS	264	8.570	4.726	36.929	1.00	0.00	N
ATOM	2312	CA	LYS	264	9.148	3.428	36.808	1.00	0.00	C
ATOM	2313	C	LYS	264	10.578	3.670	37.133	1.00	0.00	C
ATOM	2314	O	LYS	264	11.396	3.925	36.250	1.00	0.00	O
ATOM	2315	CB	LYS	264	9.070	2.837	35.390	1.00	0.00	C
ATOM	2316	CG	LYS	264	7.655	2.407	35.004	1.00	0.00	C
ATOM	2317	CD	LYS	264	7.088	1.325	35.923	1.00	0.00	C
ATOM	2318	CE	LYS	264	5.672	0.882	35.551	1.00	0.00	C
ATOM	2319	NZ	LYS	264	5.215	-0.179	36.476	1.00	0.00	N
ATOM	2320	H	LYS	264	8.493	5.352	36.115	1.00	0.00	H
ATOM	2321	HA	LYS	264	8.685	2.725	37.501	1.00	0.00	H
ATOM	2322	1HB	LYS	264	9.695	1.953	35.265	1.00	0.00	H
ATOM	2323	2HB	LYS	264	9.389	3.540	34.620	1.00	0.00	H
ATOM	2324	1HG	LYS	264	7.594	1.999	33.995	1.00	0.00	H
ATOM	2325	2HG	LYS	264	6.937	3.226	35.035	1.00	0.00	H
ATOM	2326	1HD	LYS	264	7.021	1.627	36.968	1.00	0.00	H
ATOM	2327	2HD	LYS	264	7.675	0.406	35.933	1.00	0.00	H
ATOM	2328	1HE	LYS	264	5.658	0.493	34.532	1.00	0.00	H
ATOM	2329	2HE	LYS	264	4.988	1.728	35.616	1.00	0.00	H
ATOM	2330	1HZ	LYS	264	5.956	-0.379	37.162	1.00	0.00	H
ATOM	2331	2HZ	LYS	264	4.367	0.136	36.968	1.00	0.00	H
ATOM	2332	3HZ	LYS	264	5.003	-1.033	35.941	1.00	0.00	H
ATOM	2333	N	GLU	265	10.901	3.614	38.438	1.00	0.00	N
ATOM	2334	CA	GLU	265	12.232	3.911	38.861	1.00	0.00	C
ATOM	2335	C	GLU	265	12.640	2.838	39.810	1.00	0.00	C
ATOM	2336	O	GLU	265	12.170	1.706	39.718	1.00	0.00	O
ATOM	2337	CB	GLU	265	12.346	5.273	39.569	1.00	0.00	C
ATOM	2338	CG	GLU	265	13.781	5.779	39.744	1.00	0.00	C
ATOM	2339	CD	GLU	265	14.355	6.111	38.376	1.00	0.00	C
ATOM	2340	OE1	GLU	265	13.820	5.593	37.362	1.00	0.00	O
ATOM	2341	OE2	GLU	265	15.347	6.890	38.332	1.00	0.00	O
ATOM	2342	H	GLU	265	10.186	3.356	39.133	1.00	0.00	H
ATOM	2343	HA	GLU	265	12.857	3.919	37.968	1.00	0.00	H
ATOM	2344	1HB	GLU	265	11.906	5.179	40.561	1.00	0.00	H
ATOM	2345	2HB	GLU	265	11.805	6.011	38.977	1.00	0.00	H
ATOM	2346	1HG	GLU	265	14.374	4.997	40.219	1.00	0.00	H
ATOM	2347	2HG	GLU	265	13.766	6.671	40.370	1.00	0.00	H
ATOM	2348	N	SER	266	13.547	3.167	40.747	1.00	0.00	N
ATOM	2349	CA	SER	266	14.033	2.159	41.627	1.00	0.00	C
ATOM	2350	C	SER	266	14.768	1.245	40.725	1.00	0.00	C
ATOM	2351	O	SER	266	15.774	1.622	40.125	1.00	0.00	O
ATOM	2352	CB	SER	266	12.920	1.371	42.340	1.00	0.00	C
ATOM	2353	OG	SER	266	12.204	2.227	43.218	1.00	0.00	O
ATOM	2354	H	SER	266	13.885	4.136	40.826	1.00	0.00	H
ATOM	2355	HA	SER	266	14.684	2.585	42.389	1.00	0.00	H
ATOM	2356	1HB	SER	266	13.352	0.554	42.917	1.00	0.00	H
ATOM	2357	2HB	SER	266	12.227	0.957	41.607	1.00	0.00	H
ATOM	2358	HG	SER	266	12.615	3.170	43.190	1.00	0.00	H
ATOM	2359	N	ALA	267	14.271	0.007	40.598	1.00	0.00	N
ATOM	2360	CA	ALA	267	14.900	-0.876	39.675	1.00	0.00	C
ATOM	2361	C	ALA	267	14.689	-0.281	38.319	1.00	0.00	C
ATOM	2362	O	ALA	267	15.627	-0.183	37.530	1.00	0.00	O
ATOM	2363	CB	ALA	267	14.283	-2.286	39.676	1.00	0.00	C
ATOM	2364	H	ALA	267	13.457	-0.296	41.152	1.00	0.00	H
ATOM	2365	HA	ALA	267	15.952	-0.911	39.957	1.00	0.00	H
ATOM	2366	1HB	ALA	267	13.469	-2.326	40.400	1.00	0.00	H
ATOM	2367	2HB	ALA	267	13.896	-2.514	38.682	1.00	0.00	H
ATOM	2368	3HB	ALA	267	15.045	-3.016	39.945	1.00	0.00	H
ATOM	2369	N	ALA	268	13.439	0.145	38.027	1.00	0.00	N
ATOM	2370	CA	ALA	268	13.096	0.696	36.748	1.00	0.00	C
ATOM	2371	C	ALA	268	12.964	-0.484	35.852	1.00	0.00	C
ATOM	2372	O	ALA	268	12.531	-1.550	36.284	1.00	0.00	O
ATOM	2373	CB	ALA	268	14.139	1.664	36.163	1.00	0.00	C
ATOM	2374	H	ALA	268	12.707	0.071	38.748	1.00	0.00	H
ATOM	2375	HA	ALA	268	12.159	1.226	36.917	1.00	0.00	H

ATOM	2376	1HB	ALA	268	14.977	1.756	36.853	1.00	0.00	H
ATOM	2377	2HB	ALA	268	14.496	1.279	35.207	1.00	0.00	H
ATOM	2378	3HB	ALA	268	13.683	2.642	36.012	1.00	0.00	H
ATOM	2379	N	TYR	269	13.332	-0.332	34.568	1.00	0.00	N
ATOM	2380	CA	TYR	269	13.308	-1.488	33.728	1.00	0.00	C
ATOM	2381	C	TYR	269	14.732	-1.897	33.563	1.00	0.00	C
ATOM	2382	O	TYR	269	15.522	-1.202	32.926	1.00	0.00	O
ATOM	2383	CB	TYR	269	12.681	-1.244	32.345	1.00	0.00	C
ATOM	2384	CG	TYR	269	11.233	-0.984	32.594	1.00	0.00	C
ATOM	2385	CD1	TYR	269	10.355	-2.032	32.757	1.00	0.00	C
ATOM	2386	CD2	TYR	269	10.754	0.303	32.675	1.00	0.00	C
ATOM	2387	CE1	TYR	269	9.019	-1.800	32.990	1.00	0.00	C
ATOM	2388	CE2	TYR	269	9.419	0.541	32.907	1.00	0.00	C
ATOM	2389	CZ	TYR	269	8.550	-0.511	33.065	1.00	0.00	C
ATOM	2390	OH	TYR	269	7.180	-0.270	33.304	1.00	0.00	O
ATOM	2391	H	TYR	269	13.621	0.586	34.202	1.00	0.00	H
ATOM	2392	HA	TYR	269	12.712	-2.228	34.261	1.00	0.00	H
ATOM	2393	1HB	TYR	269	12.854	-2.156	31.774	1.00	0.00	H
ATOM	2394	2HB	TYR	269	13.200	-0.380	31.930	1.00	0.00	H
ATOM	2395	HD1	TYR	269	10.722	-3.056	32.700	1.00	0.00	H
ATOM	2396	HD2	TYR	269	11.438	1.142	32.554	1.00	0.00	H
ATOM	2397	HE1	TYR	269	8.333	-2.638	33.115	1.00	0.00	H
ATOM	2398	HE2	TYR	269	9.050	1.565	32.965	1.00	0.00	H
ATOM	2399	HH	TYR	269	7.012	0.745	33.348	1.00	0.00	H
ATOM	2400	N	ILE	270	15.098	-3.047	34.160	1.00	0.00	N
ATOM	2401	CA	ILE	270	16.461	-3.480	34.110	1.00	0.00	C
ATOM	2402	C	ILE	270	16.574	-4.571	33.104	1.00	0.00	C
ATOM	2403	O	ILE	270	15.905	-5.602	33.165	1.00	0.00	O
ATOM	2404	CB	ILE	270	16.966	-4.007	35.424	1.00	0.00	C
ATOM	2405	CG1	ILE	270	16.151	-5.234	35.872	1.00	0.00	C
ATOM	2406	CG2	ILE	270	16.952	-2.849	36.435	1.00	0.00	C
ATOM	2407	CD1	ILE	270	16.781	-5.991	37.041	1.00	0.00	C
ATOM	2408	H	ILE	270	14.395	-3.616	34.653	1.00	0.00	H
ATOM	2409	HA	ILE	270	17.083	-2.632	33.822	1.00	0.00	H
ATOM	2410	HB	ILE	270	17.979	-4.377	35.269	1.00	0.00	H
ATOM	2411	1HG1	ILE	270	16.020	-5.979	35.087	1.00	0.00	H
ATOM	2412	2HG1	ILE	270	15.141	-4.988	36.202	1.00	0.00	H
ATOM	2413	1HG2	ILE	270	16.582	-1.946	35.948	1.00	0.00	H
ATOM	2414	2HG2	ILE	270	16.300	-3.103	37.270	1.00	0.00	H
ATOM	2415	3HG2	ILE	270	17.963	-2.675	36.803	1.00	0.00	H
ATOM	2416	1HD1	ILE	270	17.708	-5.499	37.335	1.00	0.00	H
ATOM	2417	2HD1	ILE	270	16.090	-5.997	37.884	1.00	0.00	H
ATOM	2418	3HD1	ILE	270	16.993	-7.016	36.738	1.00	0.00	H
ATOM	2419	N	PRO	271	17.430	-4.325	32.159	1.00	0.00	N
ATOM	2420	CA	PRO	271	17.665	-5.252	31.096	1.00	0.00	C
ATOM	2421	C	PRO	271	18.094	-6.552	31.691	1.00	0.00	C
ATOM	2422	O	PRO	271	18.881	-6.547	32.635	1.00	0.00	O
ATOM	2423	CB	PRO	271	18.797	-4.642	30.276	1.00	0.00	C
ATOM	2424	CG	PRO	271	19.610	-3.876	31.337	1.00	0.00	C
ATOM	2425	CD	PRO	271	18.552	-3.423	32.359	1.00	0.00	C
ATOM	2426	HA	PRO	271	16.738	-5.375	30.536	1.00	0.00	H
ATOM	2427	1HB	PRO	271	18.410	-3.980	29.501	1.00	0.00	H
ATOM	2428	2HB	PRO	271	19.389	-5.414	29.786	1.00	0.00	H
ATOM	2429	1HG	PRO	271	20.126	-3.025	30.891	1.00	0.00	H
ATOM	2430	2HG	PRO	271	20.358	-4.522	31.795	1.00	0.00	H
ATOM	2431	1HD	PRO	271	18.852	-3.575	33.395	1.00	0.00	H
ATOM	2432	2HD	PRO	271	18.150	-2.429	32.161	1.00	0.00	H
ATOM	2433	N	PHE	272	17.579	-7.672	31.155	1.00	0.00	N
ATOM	2434	CA	PHE	272	17.987	-8.973	31.590	1.00	0.00	C
ATOM	2435	C	PHE	272	19.382	-9.159	31.106	1.00	0.00	C
ATOM	2436	O	PHE	272	20.182	-9.874	31.707	1.00	0.00	O
ATOM	2437	CB	PHE	272	17.132	-10.094	30.977	1.00	0.00	C
ATOM	2438	CG	PHE	272	17.811	-11.395	31.241	1.00	0.00	C
ATOM	2439	CD1	PHE	272	17.702	-12.023	32.459	1.00	0.00	C
ATOM	2440	CD2	PHE	272	18.557	-11.993	30.252	1.00	0.00	C
ATOM	2441	CE1	PHE	272	18.331	-13.224	32.689	1.00	0.00	C
ATOM	2442	CE2	PHE	272	19.189	-13.194	30.473	1.00	0.00	C
ATOM	2443	CZ	PHE	272	19.076	-13.812	31.695	1.00	0.00	C

ATOM	2444	H	PHE	272	16.871	-7.591	30.410	1.00	0.00	H
ATOM	2445	HA	PHE	272	17.922	-8.967	32.678	1.00	0.00	H
ATOM	2446	1HB	PHE	272	17.050	-9.912	29.905	1.00	0.00	H
ATOM	2447	2HB	PHE	272	16.149	-10.069	31.448	1.00	0.00	H
ATOM	2448	HD1	PHE	272	17.110	-11.563	33.251	1.00	0.00	H
ATOM	2449	HD2	PHE	272	18.648	-11.508	29.280	1.00	0.00	H
ATOM	2450	HE1	PHE	272	18.238	-13.710	33.660	1.00	0.00	H
ATOM	2451	HE2	PHE	272	19.778	-13.654	29.680	1.00	0.00	H
ATOM	2452	HZ	PHE	272	19.574	-14.764	31.875	1.00	0.00	H
ATOM	2453	N	GLY	273	19.703	-8.479	29.994	1.00	0.00	N
ATOM	2454	CA	GLY	273	20.971	-8.629	29.354	1.00	0.00	C
ATOM	2455	C	GLY	273	20.614	-9.133	28.003	1.00	0.00	C
ATOM	2456	O	GLY	273	21.319	-8.908	27.020	1.00	0.00	O
ATOM	2457	H	GLY	273	19.013	-7.829	29.589	1.00	0.00	H
ATOM	2458	1HA	GLY	273	21.602	-9.333	29.895	1.00	0.00	H
ATOM	2459	2HA	GLY	273	21.499	-7.677	29.304	1.00	0.00	H
ATOM	2460	N	GLU	274	19.476	-9.846	27.948	1.00	0.00	N
ATOM	2461	CA	GLU	274	18.940	-10.319	26.713	1.00	0.00	C
ATOM	2462	C	GLU	274	18.518	-9.086	25.998	1.00	0.00	C
ATOM	2463	O	GLU	274	18.538	-9.015	24.769	1.00	0.00	O
ATOM	2464	CB	GLU	274	17.706	-11.220	26.903	1.00	0.00	C
ATOM	2465	CG	GLU	274	17.361	-12.077	25.680	1.00	0.00	C
ATOM	2466	CD	GLU	274	16.616	-11.235	24.652	1.00	0.00	C
ATOM	2467	OE1	GLU	274	16.177	-10.108	25.002	1.00	0.00	O
ATOM	2468	OE2	GLU	274	16.471	-11.719	23.497	1.00	0.00	O
ATOM	2469	H	GLU	274	18.975	-10.057	28.823	1.00	0.00	H
ATOM	2470	HA	GLU	274	19.770	-10.844	26.241	1.00	0.00	H
ATOM	2471	1HB	GLU	274	16.846	-10.584	27.115	1.00	0.00	H
ATOM	2472	2HB	GLU	274	17.899	-11.894	27.737	1.00	0.00	H
ATOM	2473	1HG	GLU	274	16.730	-12.913	25.980	1.00	0.00	H
ATOM	2474	2HG	GLU	274	18.275	-12.463	25.229	1.00	0.00	H
ATOM	2475	N	GLY	275	18.144	-8.054	26.782	1.00	0.00	N
ATOM	2476	CA	GLY	275	17.694	-6.818	26.215	1.00	0.00	C
ATOM	2477	C	GLY	275	16.234	-6.719	26.466	1.00	0.00	C
ATOM	2478	O	GLY	275	15.637	-5.654	26.331	1.00	0.00	O
ATOM	2479	H	GLY	275	18.182	-8.156	27.806	1.00	0.00	H
ATOM	2480	1HA	GLY	275	17.913	-6.849	25.147	1.00	0.00	H
ATOM	2481	2HA	GLY	275	18.238	-6.014	26.710	1.00	0.00	H
ATOM	2482	N	ASP	276	15.608	-7.849	26.850	1.00	0.00	N
ATOM	2483	CA	ASP	276	14.200	-7.829	27.109	1.00	0.00	C
ATOM	2484	C	ASP	276	14.038	-7.181	28.442	1.00	0.00	C
ATOM	2485	O	ASP	276	15.007	-6.698	29.028	1.00	0.00	O
ATOM	2486	CB	ASP	276	13.559	-9.214	27.167	1.00	0.00	C
ATOM	2487	CG	ASP	276	13.557	-9.785	25.755	1.00	0.00	C
ATOM	2488	OD1	ASP	276	13.760	-8.986	24.800	1.00	0.00	O
ATOM	2489	OD2	ASP	276	13.354	-11.023	25.614	1.00	0.00	O
ATOM	2490	H	ASP	276	16.140	-8.724	26.956	1.00	0.00	H
ATOM	2491	HA	ASP	276	13.755	-7.248	26.301	1.00	0.00	H
ATOM	2492	1HB	ASP	276	12.543	-9.095	27.543	1.00	0.00	H
ATOM	2493	2HB	ASP	276	14.157	-9.829	27.838	1.00	0.00	H
ATOM	2494	N	PHE	277	12.795	-7.146	28.960	1.00	0.00	N
ATOM	2495	CA	PHE	277	12.576	-6.530	30.226	1.00	0.00	C
ATOM	2496	C	PHE	277	12.671	-7.611	31.252	1.00	0.00	C
ATOM	2497	O	PHE	277	11.708	-8.342	31.486	1.00	0.00	O
ATOM	2498	CB	PHE	277	11.166	-5.929	30.358	1.00	0.00	C
ATOM	2499	CG	PHE	277	11.010	-4.919	29.273	1.00	0.00	C
ATOM	2500	CD1	PHE	277	10.651	-5.319	28.006	1.00	0.00	C
ATOM	2501	CD2	PHE	277	11.226	-3.581	29.513	1.00	0.00	C
ATOM	2502	CE1	PHE	277	10.506	-4.402	26.992	1.00	0.00	C
ATOM	2503	CE2	PHE	277	11.083	-2.659	28.502	1.00	0.00	C
ATOM	2504	CZ	PHE	277	10.722	-3.068	27.240	1.00	0.00	C
ATOM	2505	H	PHE	277	12.007	-7.562	28.443	1.00	0.00	H
ATOM	2506	HA	PHE	277	13.356	-5.779	30.348	1.00	0.00	H
ATOM	2507	1HB	PHE	277	11.099	-5.469	31.344	1.00	0.00	H
ATOM	2508	2HB	PHE	277	10.452	-6.746	30.248	1.00	0.00	H
ATOM	2509	HD1	PHE	277	10.479	-6.376	27.803	1.00	0.00	H
ATOM	2510	HD2	PHE	277	11.512	-3.249	30.511	1.00	0.00	H
ATOM	2511	HE1	PHE	277	10.220	-4.732	25.993	1.00	0.00	H

ATOM	2512	HE2	PHE	277	11.256	-1.601	28.702	1.00	0.00	H
ATOM	2513	HZ	PHE	277	10.607	-2.337	26.439	1.00	0.00	H
ATOM	2514	N	TYR	278	13.860	-7.772	31.864	1.00	0.00	N
ATOM	2515	CA	TYR	278	13.996	-8.805	32.842	1.00	0.00	C
ATOM	2516	C	TYR	278	13.234	-8.444	34.075	1.00	0.00	C
ATOM	2517	O	TYR	278	12.479	-9.261	34.604	1.00	0.00	O
ATOM	2518	CB	TYR	278	15.446	-9.075	33.265	1.00	0.00	C
ATOM	2519	CG	TYR	278	15.368	-10.173	34.268	1.00	0.00	C
ATOM	2520	CD1	TYR	278	15.168	-11.468	33.857	1.00	0.00	C
ATOM	2521	CD2	TYR	278	15.494	-9.912	35.614	1.00	0.00	C
ATOM	2522	CE1	TYR	278	15.092	-12.493	34.766	1.00	0.00	C
ATOM	2523	CE2	TYR	278	15.419	-10.935	36.532	1.00	0.00	C
ATOM	2524	CZ	TYR	278	15.217	-12.228	36.107	1.00	0.00	C
ATOM	2525	OH	TYR	278	15.140	-13.277	37.047	1.00	0.00	O
ATOM	2526	H	TYR	278	14.656	-7.161	31.631	1.00	0.00	H
ATOM	2527	HA	TYR	278	13.607	-9.744	32.448	1.00	0.00	H
ATOM	2528	1HB	TYR	278	15.805	-8.135	33.684	1.00	0.00	H
ATOM	2529	2HB	TYR	278	15.965	-9.364	32.351	1.00	0.00	H
ATOM	2530	HD1	TYR	278	15.068	-11.684	32.793	1.00	0.00	H
ATOM	2531	HD2	TYR	278	15.654	-8.889	35.954	1.00	0.00	H
ATOM	2532	HE1	TYR	278	14.932	-13.515	34.423	1.00	0.00	H
ATOM	2533	HE2	TYR	278	15.519	-10.720	37.596	1.00	0.00	H
ATOM	2534	HH	TYR	278	14.399	-13.070	37.732	1.00	0.00	H
ATOM	2535	N	TYR	279	13.398	-7.197	34.562	1.00	0.00	N
ATOM	2536	CA	TYR	279	12.758	-6.824	35.794	1.00	0.00	C
ATOM	2537	C	TYR	279	12.053	-5.524	35.575	1.00	0.00	C
ATOM	2538	O	TYR	279	12.429	-4.747	34.697	1.00	0.00	O
ATOM	2539	CB	TYR	279	13.767	-6.632	36.943	1.00	0.00	C
ATOM	2540	CG	TYR	279	13.033	-6.261	38.186	1.00	0.00	C
ATOM	2541	CD1	TYR	279	12.472	-7.237	38.976	1.00	0.00	C
ATOM	2542	CD2	TYR	279	12.914	-4.944	38.571	1.00	0.00	C
ATOM	2543	CE1	TYR	279	11.797	-6.907	40.130	1.00	0.00	C
ATOM	2544	CE2	TYR	279	12.242	-4.608	39.722	1.00	0.00	C
ATOM	2545	CZ	TYR	279	11.681	-5.589	40.503	1.00	0.00	C
ATOM	2546	OH	TYR	279	10.992	-5.247	41.685	1.00	0.00	O
ATOM	2547	H	TYR	279	13.979	-6.515	34.053	1.00	0.00	H
ATOM	2548	HA	TYR	279	12.050	-7.609	36.058	1.00	0.00	H
ATOM	2549	1HB	TYR	279	14.466	-5.838	36.679	1.00	0.00	H
ATOM	2550	2HB	TYR	279	14.311	-7.562	37.102	1.00	0.00	H
ATOM	2551	HD1	TYR	279	12.562	-8.283	38.685	1.00	0.00	H
ATOM	2552	HD2	TYR	279	13.357	-4.160	37.956	1.00	0.00	H
ATOM	2553	HE1	TYR	279	11.355	-7.689	40.746	1.00	0.00	H
ATOM	2554	HE2	TYR	279	12.154	-3.561	40.015	1.00	0.00	H
ATOM	2555	HH	TYR	279	11.059	-4.231	41.840	1.00	0.00	H
ATOM	2556	N	HIS	280	10.989	-5.267	36.363	1.00	0.00	N
ATOM	2557	CA	HIS	280	10.235	-4.059	36.201	1.00	0.00	C
ATOM	2558	C	HIS	280	10.105	-3.437	37.556	1.00	0.00	C
ATOM	2559	O	HIS	280	9.822	-4.127	38.534	1.00	0.00	O
ATOM	2560	CB	HIS	280	8.801	-4.330	35.718	1.00	0.00	C
ATOM	2561	CG	HIS	280	8.752	-5.281	34.558	1.00	0.00	C
ATOM	2562	ND1	HIS	280	8.694	-6.650	34.703	1.00	0.00	N
ATOM	2563	CD2	HIS	280	8.759	-5.050	33.217	1.00	0.00	C
ATOM	2564	CE1	HIS	280	8.669	-7.176	33.453	1.00	0.00	C
ATOM	2565	NE2	HIS	280	8.707	-6.244	32.518	1.00	0.00	N
ATOM	2566	H	HIS	280	10.715	-5.945	37.088	1.00	0.00	H
ATOM	2567	HA	HIS	280	10.794	-3.421	35.516	1.00	0.00	H
ATOM	2568	1HB	HIS	280	8.290	-3.424	35.388	1.00	0.00	H
ATOM	2569	2HB	HIS	280	8.172	-4.766	36.494	1.00	0.00	H
ATOM	2570	HD1	HIS	280	8.673	-7.173	35.590	1.00	0.00	H
ATOM	2571	HD2	HIS	280	8.799	-4.062	32.757	1.00	0.00	H
ATOM	2572	HE1	HIS	280	8.622	-8.244	33.244	1.00	0.00	H
ATOM	2573	HE2	HIS	280	8.699	-6.376	31.496	1.00	0.00	H
ATOM	2574	N	ALA	281	10.314	-2.108	37.663	1.00	0.00	N
ATOM	2575	CA	ALA	281	10.175	-1.508	38.958	1.00	0.00	C
ATOM	2576	C	ALA	281	9.410	-0.232	38.819	1.00	0.00	C
ATOM	2577	O	ALA	281	9.697	0.591	37.950	1.00	0.00	O
ATOM	2578	CB	ALA	281	11.516	-1.162	39.624	1.00	0.00	C
ATOM	2579	H	ALA	281	10.565	-1.542	36.839	1.00	0.00	H

```
ATOM   2580  HA  ALA   281       9.638  -2.197  39.609  1.00  0.00           H
ATOM   2581 1HB  ALA   281      12.334  -1.448  38.963  1.00  0.00           H
ATOM   2582 2HB  ALA   281      11.561  -0.089  39.814  1.00  0.00           H
ATOM   2583 3HB  ALA   281      11.604  -1.702  40.566  1.00  0.00           H
ATOM   2584  N   ALA   282       8.394  -0.044  39.684  1.00  0.00           N
ATOM   2585  CA  ALA   282       7.641   1.175  39.659  1.00  0.00           C
ATOM   2586  C   ALA   282       7.535   1.640  41.070  1.00  0.00           C
ATOM   2587  O   ALA   282       7.371   0.838  41.987  1.00  0.00           O
ATOM   2588  CB  ALA   282       6.206   1.006  39.131  1.00  0.00           C
ATOM   2589  H   ALA   282       8.157  -0.779  40.365  1.00  0.00           H
ATOM   2590  HA  ALA   282       8.199   1.874  39.036  1.00  0.00           H
ATOM   2591 1HB  ALA   282       6.034  -0.038  38.870  1.00  0.00           H
ATOM   2592 2HB  ALA   282       5.496   1.308  39.901  1.00  0.00           H
ATOM   2593 3HB  ALA   282       6.068   1.627  38.246  1.00  0.00           H
ATOM   2594  N   ILE   283       7.655   2.960  41.291  1.00  0.00           N
ATOM   2595  CA  ILE   283       7.501   3.417  42.634  1.00  0.00           C
ATOM   2596  C   ILE   283       6.273   4.261  42.670  1.00  0.00           C
ATOM   2597  O   ILE   283       6.094   5.159  41.847  1.00  0.00           O
ATOM   2598  CB  ILE   283       8.655   4.217  43.170  1.00  0.00           C
ATOM   2599  CG1 ILE   283       8.501   4.389  44.691  1.00  0.00           C
ATOM   2600  CG2 ILE   283       8.755   5.538  42.391  1.00  0.00           C
ATOM   2601  CD1 ILE   283       9.765   4.892  45.386  1.00  0.00           C
ATOM   2602  H   ILE   283       7.850   3.616  40.521  1.00  0.00           H
ATOM   2603  HA  ILE   283       7.402   2.532  43.263  1.00  0.00           H
ATOM   2604  HB  ILE   283       9.573   3.643  43.046  1.00  0.00           H
ATOM   2605 1HG1 ILE   283       8.243   3.468  45.214  1.00  0.00           H
ATOM   2606 2HG1 ILE   283       7.724   5.098  44.977  1.00  0.00           H
ATOM   2607 1HG2 ILE   283       7.967   5.577  41.638  1.00  0.00           H
ATOM   2608 2HG2 ILE   283       8.641   6.375  43.079  1.00  0.00           H
ATOM   2609 3HG2 ILE   283       9.727   5.599  41.901  1.00  0.00           H
ATOM   2610 1HD1 ILE   283      10.553   5.035  44.647  1.00  0.00           H
ATOM   2611 2HD1 ILE   283       9.555   5.839  45.881  1.00  0.00           H
ATOM   2612 3HD1 ILE   283      10.089   4.160  46.125  1.00  0.00           H
ATOM   2613  N   PHE   284       5.379   3.963  43.629  1.00  0.00           N
ATOM   2614  CA  PHE   284       4.153   4.691  43.748  1.00  0.00           C
ATOM   2615  C   PHE   284       4.420   5.967  44.469  1.00  0.00           C
ATOM   2616  O   PHE   284       5.515   6.204  44.978  1.00  0.00           O
ATOM   2617  CB  PHE   284       3.069   3.986  44.587  1.00  0.00           C
ATOM   2618  CG  PHE   284       2.427   2.887  43.816  1.00  0.00           C
ATOM   2619  CD1 PHE   284       3.011   1.645  43.722  1.00  0.00           C
ATOM   2620  CD2 PHE   284       1.215   3.104  43.202  1.00  0.00           C
ATOM   2621  CE1 PHE   284       2.397   0.640  43.012  1.00  0.00           C
ATOM   2622  CE2 PHE   284       0.596   2.103  42.491  1.00  0.00           C
ATOM   2623  CZ  PHE   284       1.189   0.867  42.395  1.00  0.00           C
ATOM   2624  H   PHE   284       5.580   3.198  44.288  1.00  0.00           H
ATOM   2625  HA  PHE   284       3.768   4.898  42.749  1.00  0.00           H
ATOM   2626 1HB  PHE   284       2.288   4.685  44.885  1.00  0.00           H
ATOM   2627 2HB  PHE   284       3.494   3.554  45.493  1.00  0.00           H
ATOM   2628  HD1 PHE   284       3.965   1.456  44.213  1.00  0.00           H
ATOM   2629  HD2 PHE   284       0.739   4.081  43.280  1.00  0.00           H
ATOM   2630  HE1 PHE   284       2.869  -0.339  42.938  1.00  0.00           H
ATOM   2631  HE2 PHE   284      -0.361   2.289  42.005  1.00  0.00           H
ATOM   2632  HZ  PHE   284       0.703   0.069  41.832  1.00  0.00           H
ATOM   2633  N   GLY   285       3.397   6.842  44.485  1.00  0.00           N
ATOM   2634  CA  GLY   285       3.440   8.052  45.247  1.00  0.00           C
ATOM   2635  C   GLY   285       2.218   7.984  46.105  1.00  0.00           C
ATOM   2636  O   GLY   285       1.216   8.645  45.834  1.00  0.00           O
ATOM   2637  H   GLY   285       2.554   6.633  43.929  1.00  0.00           H
ATOM   2638 1HA  GLY   285       3.416   8.839  44.494  1.00  0.00           H
ATOM   2639 2HA  GLY   285       4.378   7.985  45.797  1.00  0.00           H
ATOM   2640  N   GLY   286       2.279   7.135  47.151  1.00  0.00           N
ATOM   2641  CA  GLY   286       1.177   6.887  48.036  1.00  0.00           C
ATOM   2642  C   GLY   286       0.923   8.016  48.986  1.00  0.00           C
ATOM   2643  O   GLY   286      -0.225   8.408  49.189  1.00  0.00           O
ATOM   2644  H   GLY   286       3.164   6.637  47.324  1.00  0.00           H
ATOM   2645 1HA  GLY   286       1.320   6.004  48.659  1.00  0.00           H
ATOM   2646 2HA  GLY   286       0.235   6.726  47.510  1.00  0.00           H
ATOM   2647  N   THR   287       1.982   8.558  49.621  1.00  0.00           N
```

ATOM	2648	CA	THR	287	1.737	9.563	50.617	1.00	0.00	C
ATOM	2649	C	THR	287	2.959	10.420	50.730	1.00	0.00	C
ATOM	2650	O	THR	287	3.998	10.130	50.140	1.00	0.00	O
ATOM	2651	CB	THR	287	1.472	8.963	51.971	1.00	0.00	C
ATOM	2652	OG1	THR	287	0.994	9.942	52.881	1.00	0.00	O
ATOM	2653	CG2	THR	287	2.779	8.343	52.493	1.00	0.00	C
ATOM	2654	H	THR	287	2.941	8.258	49.397	1.00	0.00	H
ATOM	2655	HA	THR	287	0.879	10.156	50.300	1.00	0.00	H
ATOM	2656	HB	THR	287	0.703	8.197	51.864	1.00	0.00	H
ATOM	2657	HG1	THR	287	1.547	10.804	52.780	1.00	0.00	H
ATOM	2658	1HG2	THR	287	3.570	8.490	51.758	1.00	0.00	H
ATOM	2659	2HG2	THR	287	3.060	8.823	53.430	1.00	0.00	H
ATOM	2660	3HG2	THR	287	2.633	7.275	52.661	1.00	0.00	H
ATOM	2661	N	PRO	288	2.838	11.501	51.452	1.00	0.00	N
ATOM	2662	CA	PRO	288	3.990	12.335	51.656	1.00	0.00	C
ATOM	2663	C	PRO	288	4.929	11.677	52.612	1.00	0.00	C
ATOM	2664	O	PRO	288	4.465	10.951	53.489	1.00	0.00	O
ATOM	2665	CB	PRO	288	3.458	13.680	52.144	1.00	0.00	C
ATOM	2666	CG	PRO	288	2.056	13.759	51.515	1.00	0.00	C
ATOM	2667	CD	PRO	288	1.618	12.292	51.375	1.00	0.00	C
ATOM	2668	HA	PRO	288	4.502	12.496	50.707	1.00	0.00	H
ATOM	2669	1HB	PRO	288	4.097	14.497	51.810	1.00	0.00	H
ATOM	2670	2HB	PRO	288	3.414	13.711	53.232	1.00	0.00	H
ATOM	2671	1HG	PRO	288	2.214	14.268	50.564	1.00	0.00	H
ATOM	2672	2HG	PRO	288	1.469	14.331	52.233	1.00	0.00	H
ATOM	2673	1HD	PRO	288	0.991	11.958	52.202	1.00	0.00	H
ATOM	2674	2HD	PRO	288	1.180	12.073	50.400	1.00	0.00	H
ATOM	2675	N	THR	289	6.250	11.901	52.461	1.00	0.00	N
ATOM	2676	CA	THR	289	7.166	11.281	53.373	1.00	0.00	C
ATOM	2677	C	THR	289	8.535	11.823	53.093	1.00	0.00	C
ATOM	2678	O	THR	289	8.677	12.880	52.479	1.00	0.00	O
ATOM	2679	CB	THR	289	7.214	9.785	53.233	1.00	0.00	C
ATOM	2680	OG1	THR	289	7.893	9.199	54.335	1.00	0.00	O
ATOM	2681	CG2	THR	289	7.927	9.436	51.916	1.00	0.00	C
ATOM	2682	H	THR	289	6.595	12.507	51.703	1.00	0.00	H
ATOM	2683	HA	THR	289	6.849	11.527	54.386	1.00	0.00	H
ATOM	2684	HB	THR	289	6.193	9.402	53.222	1.00	0.00	H
ATOM	2685	HG1	THR	289	7.656	9.711	55.196	1.00	0.00	H
ATOM	2686	1HG2	THR	289	8.222	10.353	51.407	1.00	0.00	H
ATOM	2687	2HG2	THR	289	8.813	8.838	52.129	1.00	0.00	H
ATOM	2688	3HG2	THR	289	7.251	8.868	51.276	1.00	0.00	H
ATOM	2689	N	GLN	290	9.578	11.106	53.571	1.00	0.00	N
ATOM	2690	CA	GLN	290	10.946	11.488	53.362	1.00	0.00	C
ATOM	2691	C	GLN	290	11.307	11.065	51.975	1.00	0.00	C
ATOM	2692	O	GLN	290	11.184	9.898	51.607	1.00	0.00	O
ATOM	2693	CB	GLN	290	11.927	10.823	54.345	1.00	0.00	C
ATOM	2694	CG	GLN	290	11.799	11.334	55.783	1.00	0.00	C
ATOM	2695	CD	GLN	290	12.408	12.729	55.844	1.00	0.00	C
ATOM	2696	OE1	GLN	290	12.950	13.230	54.860	1.00	0.00	O
ATOM	2697	NE2	GLN	290	12.323	13.376	57.038	1.00	0.00	N
ATOM	2698	H	GLN	290	9.382	10.249	54.108	1.00	0.00	H
ATOM	2699	HA	GLN	290	10.994	12.570	53.483	1.00	0.00	H
ATOM	2700	1HB	GLN	290	12.975	10.972	54.086	1.00	0.00	H
ATOM	2701	2HB	GLN	290	11.807	9.742	54.419	1.00	0.00	H
ATOM	2702	1HG	GLN	290	12.337	10.646	56.434	1.00	0.00	H
ATOM	2703	2HG	GLN	290	10.739	11.361	56.038	1.00	0.00	H
ATOM	2704	1HE2	GLN	290	12.721	14.320	57.141	1.00	0.00	H
ATOM	2705	2HE2	GLN	290	11.860	12.921	57.838	1.00	0.00	H
ATOM	2706	N	VAL	291	11.752	12.047	51.171	1.00	0.00	N
ATOM	2707	CA	VAL	291	12.052	11.906	49.776	1.00	0.00	C
ATOM	2708	C	VAL	291	13.310	11.142	49.519	1.00	0.00	C
ATOM	2709	O	VAL	291	13.433	10.541	48.453	1.00	0.00	O
ATOM	2710	CB	VAL	291	12.204	13.227	49.097	1.00	0.00	C
ATOM	2711	CG1	VAL	291	10.858	13.966	49.175	1.00	0.00	C
ATOM	2712	CG2	VAL	291	13.372	13.971	49.761	1.00	0.00	C
ATOM	2713	H	VAL	291	11.888	12.977	51.592	1.00	0.00	H
ATOM	2714	HA	VAL	291	11.274	11.382	49.220	1.00	0.00	H
ATOM	2715	HB	VAL	291	12.484	13.047	48.059	1.00	0.00	H

ATOM	2716	1HG1	VAL	291	10.132	13.346	49.702	1.00	0.00	H
ATOM	2717	2HG1	VAL	291	10.989	14.906	49.710	1.00	0.00	H
ATOM	2718	3HG1	VAL	291	10.495	14.169	48.167	1.00	0.00	H
ATOM	2719	1HG2	VAL	291	13.793	13.353	50.554	1.00	0.00	H
ATOM	2720	2HG2	VAL	291	14.140	14.179	49.016	1.00	0.00	H
ATOM	2721	3HG2	VAL	291	13.012	14.909	50.183	1.00	0.00	H
ATOM	2722	N	LEU	292	14.277	11.164	50.462	1.00	0.00	N
ATOM	2723	CA	LEU	292	15.569	10.575	50.237	1.00	0.00	C
ATOM	2724	C	LEU	292	15.457	9.193	49.670	1.00	0.00	C
ATOM	2725	O	LEU	292	14.870	8.285	50.255	1.00	0.00	O
ATOM	2726	CB	LEU	292	16.488	10.588	51.485	1.00	0.00	C
ATOM	2727	CG	LEU	292	15.978	9.868	52.755	1.00	0.00	C
ATOM	2728	CD1	LEU	292	14.588	10.374	53.161	1.00	0.00	C
ATOM	2729	CD2	LEU	292	16.112	8.339	52.686	1.00	0.00	C
ATOM	2730	H	LEU	292	14.083	11.615	51.367	1.00	0.00	H
ATOM	2731	HA	LEU	292	16.163	11.162	49.537	1.00	0.00	H
ATOM	2732	1HB	LEU	292	16.648	11.629	51.762	1.00	0.00	H
ATOM	2733	2HB	LEU	292	17.423	10.102	51.208	1.00	0.00	H
ATOM	2734	HG	LEU	292	16.648	10.032	53.598	1.00	0.00	H
ATOM	2735	1HD1	LEU	292	14.259	11.139	52.457	1.00	0.00	H
ATOM	2736	2HD1	LEU	292	13.881	9.544	53.150	1.00	0.00	H
ATOM	2737	3HD1	LEU	292	14.634	10.798	54.163	1.00	0.00	H
ATOM	2738	1HD2	LEU	292	16.551	8.055	51.730	1.00	0.00	H
ATOM	2739	2HD2	LEU	292	16.752	7.992	53.497	1.00	0.00	H
ATOM	2740	3HD2	LEU	292	15.126	7.882	52.781	1.00	0.00	H
ATOM	2741	N	ASN	293	15.983	9.054	48.437	1.00	0.00	N
ATOM	2742	CA	ASN	293	16.061	7.821	47.709	1.00	0.00	C
ATOM	2743	C	ASN	293	14.705	7.432	47.211	1.00	0.00	C
ATOM	2744	O	ASN	293	14.585	6.761	46.187	1.00	0.00	O
ATOM	2745	CB	ASN	293	16.617	6.667	48.565	1.00	0.00	C
ATOM	2746	CG	ASN	293	16.899	5.473	47.662	1.00	0.00	C
ATOM	2747	OD1	ASN	293	15.993	4.858	47.102	1.00	0.00	O
ATOM	2748	ND2	ASN	293	18.208	5.136	47.513	1.00	0.00	N
ATOM	2749	H	ASN	293	16.358	9.898	47.982	1.00	0.00	H
ATOM	2750	HA	ASN	293	16.731	7.931	46.856	1.00	0.00	H
ATOM	2751	1HB	ASN	293	15.877	6.397	49.319	1.00	0.00	H
ATOM	2752	2HB	ASN	293	17.537	6.995	49.046	1.00	0.00	H
ATOM	2753	1HD2	ASN	293	18.469	4.340	46.913	1.00	0.00	H
ATOM	2754	2HD2	ASN	293	18.937	5.676	47.999	1.00	0.00	H
ATOM	2755	N	ILE	294	13.638	7.863	47.904	1.00	0.00	N
ATOM	2756	CA	ILE	294	12.326	7.463	47.488	1.00	0.00	C
ATOM	2757	C	ILE	294	11.915	8.198	46.246	1.00	0.00	C
ATOM	2758	O	ILE	294	11.329	7.610	45.338	1.00	0.00	O
ATOM	2759	CB	ILE	294	11.275	7.676	48.544	1.00	0.00	C
ATOM	2760	CG1	ILE	294	9.992	6.906	48.184	1.00	0.00	C
ATOM	2761	CG2	ILE	294	11.064	9.187	48.729	1.00	0.00	C
ATOM	2762	CD1	ILE	294	9.010	6.779	49.349	1.00	0.00	C
ATOM	2763	H	ILE	294	13.761	8.473	48.724	1.00	0.00	H
ATOM	2764	HA	ILE	294	12.297	6.394	47.275	1.00	0.00	H
ATOM	2765	HB	ILE	294	11.620	7.225	49.474	1.00	0.00	H
ATOM	2766	1HG1	ILE	294	10.176	5.883	47.854	1.00	0.00	H
ATOM	2767	2HG1	ILE	294	9.420	7.366	47.378	1.00	0.00	H
ATOM	2768	1HG2	ILE	294	11.723	9.731	48.053	1.00	0.00	H
ATOM	2769	2HG2	ILE	294	10.027	9.439	48.505	1.00	0.00	H
ATOM	2770	3HG2	ILE	294	11.291	9.462	49.758	1.00	0.00	H
ATOM	2771	1HD1	ILE	294	9.423	7.272	50.228	1.00	0.00	H
ATOM	2772	2HD1	ILE	294	8.064	7.249	49.080	1.00	0.00	H
ATOM	2773	3HD1	ILE	294	8.841	5.724	49.569	1.00	0.00	H
ATOM	2774	N	THR	295	12.229	9.505	46.162	1.00	0.00	N
ATOM	2775	CA	THR	295	11.793	10.311	45.055	1.00	0.00	C
ATOM	2776	C	THR	295	12.858	10.330	44.009	1.00	0.00	C
ATOM	2777	O	THR	295	13.954	9.813	44.216	1.00	0.00	O
ATOM	2778	CB	THR	295	11.534	11.733	45.450	1.00	0.00	C
ATOM	2779	OG1	THR	295	12.727	12.310	45.957	1.00	0.00	O
ATOM	2780	CG2	THR	295	10.429	11.764	46.521	1.00	0.00	C
ATOM	2781	H	THR	295	12.794	9.936	46.907	1.00	0.00	H
ATOM	2782	HA	THR	295	10.878	9.887	44.639	1.00	0.00	H
ATOM	2783	HB	THR	295	11.214	12.294	44.571	1.00	0.00	H

ATOM	2784	HG1	THR	295	13.410	12.412	45.193	1.00	0.00	H
ATOM	2785	1HG2	THR	295	10.100	10.746	46.734	1.00	0.00	H
ATOM	2786	2HG2	THR	295	10.818	12.218	47.432	1.00	0.00	H
ATOM	2787	3HG2	THR	295	9.584	12.348	46.155	1.00	0.00	H
ATOM	2788	N	GLN	296	12.554	10.945	42.843	1.00	0.00	N
ATOM	2789	CA	GLN	296	13.513	10.934	41.777	1.00	0.00	C
ATOM	2790	C	GLN	296	13.855	12.321	41.328	1.00	0.00	C
ATOM	2791	O	GLN	296	13.503	13.320	41.952	1.00	0.00	O
ATOM	2792	CB	GLN	296	13.059	10.149	40.537	1.00	0.00	C
ATOM	2793	CG	GLN	296	12.877	8.659	40.827	1.00	0.00	C
ATOM	2794	CD	GLN	296	14.158	8.135	41.460	1.00	0.00	C
ATOM	2795	OE1	GLN	296	14.149	7.631	42.583	1.00	0.00	O
ATOM	2796	NE2	GLN	296	15.289	8.241	40.712	1.00	0.00	N
ATOM	2797	H	GLN	296	11.645	11.415	42.722	1.00	0.00	H
ATOM	2798	HA	GLN	296	14.443	10.453	42.078	1.00	0.00	H
ATOM	2799	1HB	GLN	296	13.774	10.219	39.717	1.00	0.00	H
ATOM	2800	2HB	GLN	296	12.106	10.506	40.146	1.00	0.00	H
ATOM	2801	1HG	GLN	296	12.678	8.148	39.884	1.00	0.00	H
ATOM	2802	2HG	GLN	296	12.036	8.543	41.510	1.00	0.00	H
ATOM	2803	1HE2	GLN	296	16.185	7.891	41.081	1.00	0.00	H
ATOM	2804	2HE2	GLN	296	15.249	8.670	39.776	1.00	0.00	H
ATOM	2805	N	GLU	297	14.554	12.362	40.176	1.00	0.00	N
ATOM	2806	CA	GLU	297	15.187	13.472	39.516	1.00	0.00	C
ATOM	2807	C	GLU	297	14.220	14.506	39.044	1.00	0.00	C
ATOM	2808	O	GLU	297	14.611	15.656	38.850	1.00	0.00	O
ATOM	2809	CB	GLU	297	15.974	13.048	38.267	1.00	0.00	C
ATOM	2810	CG	GLU	297	15.075	12.505	37.152	1.00	0.00	C
ATOM	2811	CD	GLU	297	15.952	12.171	35.955	1.00	0.00	C
ATOM	2812	OE1	GLU	297	16.938	11.409	36.142	1.00	0.00	O
ATOM	2813	OE2	GLU	297	15.653	12.677	34.841	1.00	0.00	O
ATOM	2814	H	GLU	297	14.649	11.457	39.693	1.00	0.00	H
ATOM	2815	HA	GLU	297	15.893	14.004	40.152	1.00	0.00	H
ATOM	2816	1HB	GLU	297	16.702	12.263	38.470	1.00	0.00	H
ATOM	2817	2HB	GLU	297	16.537	13.868	37.822	1.00	0.00	H
ATOM	2818	1HG	GLU	297	14.348	13.275	36.894	1.00	0.00	H
ATOM	2819	2HG	GLU	297	14.573	11.611	37.523	1.00	0.00	H
ATOM	2820	N	CYS	298	12.944	14.139	38.848	1.00	0.00	N
ATOM	2821	CA	CYS	298	11.986	14.986	38.195	1.00	0.00	C
ATOM	2822	C	CYS	298	11.981	16.390	38.760	1.00	0.00	C
ATOM	2823	O	CYS	298	11.900	17.327	37.968	1.00	0.00	O
ATOM	2824	CB	CYS	298	10.550	14.445	38.303	1.00	0.00	C
ATOM	2825	SG	CYS	298	9.335	15.519	37.481	1.00	0.00	S
ATOM	2826	H	CYS	298	12.639	13.212	39.179	1.00	0.00	H
ATOM	2827	HA	CYS	298	12.179	15.083	37.126	1.00	0.00	H
ATOM	2828	1HB	CYS	298	10.216	14.344	39.335	1.00	0.00	H
ATOM	2829	2HB	CYS	298	10.438	13.459	37.851	1.00	0.00	H
ATOM	2830	HG	CYS	298	9.782	16.782	37.481	1.00	0.00	H
ATOM	2831	N	PHE	299	12.054	16.616	40.098	1.00	0.00	N
ATOM	2832	CA	PHE	299	12.065	17.995	40.533	1.00	0.00	C
ATOM	2833	C	PHE	299	12.861	18.123	41.799	1.00	0.00	C
ATOM	2834	O	PHE	299	14.090	18.050	41.787	1.00	0.00	O
ATOM	2835	CB	PHE	299	10.656	18.565	40.804	1.00	0.00	C
ATOM	2836	CG	PHE	299	10.768	20.044	41.001	1.00	0.00	C
ATOM	2837	CD1	PHE	299	11.026	20.869	39.930	1.00	0.00	C
ATOM	2838	CD2	PHE	299	10.589	20.618	42.240	1.00	0.00	C
ATOM	2839	CE1	PHE	299	11.124	22.231	40.096	1.00	0.00	C
ATOM	2840	CE2	PHE	299	10.687	21.978	42.414	1.00	0.00	C
ATOM	2841	CZ	PHE	299	10.958	22.789	41.340	1.00	0.00	C
ATOM	2842	H	PHE	299	12.099	15.839	40.772	1.00	0.00	H
ATOM	2843	HA	PHE	299	12.515	18.621	39.763	1.00	0.00	H
ATOM	2844	1HB	PHE	299	10.256	18.093	41.701	1.00	0.00	H
ATOM	2845	2HB	PHE	299	10.020	18.345	39.946	1.00	0.00	H
ATOM	2846	HD1	PHE	299	11.154	20.437	38.937	1.00	0.00	H
ATOM	2847	HD2	PHE	299	10.365	19.983	43.097	1.00	0.00	H
ATOM	2848	HE1	PHE	299	11.334	22.869	39.237	1.00	0.00	H
ATOM	2849	HE2	PHE	299	10.549	22.412	43.404	1.00	0.00	H
ATOM	2850	HZ	PHE	299	11.040	23.867	41.473	1.00	0.00	H
ATOM	2851	N	LYS	300	12.152	18.377	42.919	1.00	0.00	N

ATOM	2852	CA	LYS	300	12.711	18.546	44.231	1.00	0.00	C
ATOM	2853	C	LYS	300	11.842	19.526	44.938	1.00	0.00	C
ATOM	2854	O	LYS	300	10.626	19.541	44.767	1.00	0.00	O
ATOM	2855	CB	LYS	300	14.135	19.134	44.286	1.00	0.00	C
ATOM	2856	CG	LYS	300	14.273	20.503	43.618	1.00	0.00	C
ATOM	2857	CD	LYS	300	15.543	21.248	44.032	1.00	0.00	C
ATOM	2858	CE	LYS	300	15.398	22.016	45.347	1.00	0.00	C
ATOM	2859	NZ	LYS	300	15.336	21.070	46.484	1.00	0.00	N
ATOM	2860	H	LYS	300	11.129	18.455	42.825	1.00	0.00	H
ATOM	2861	HA	LYS	300	12.695	17.563	44.703	1.00	0.00	H
ATOM	2862	1HB	LYS	300	14.809	18.446	43.776	1.00	0.00	H
ATOM	2863	2HB	LYS	300	14.419	19.245	45.332	1.00	0.00	H
ATOM	2864	1HG	LYS	300	13.448	21.177	43.850	1.00	0.00	H
ATOM	2865	2HG	LYS	300	14.307	20.446	42.530	1.00	0.00	H
ATOM	2866	1HD	LYS	300	15.868	21.989	43.302	1.00	0.00	H
ATOM	2867	2HD	LYS	300	16.402	20.593	44.177	1.00	0.00	H
ATOM	2868	1HE	LYS	300	14.485	22.611	45.334	1.00	0.00	H
ATOM	2869	2HE	LYS	300	16.250	22.680	45.488	1.00	0.00	H
ATOM	2870	1HZ	LYS	300	15.404	20.104	46.132	1.00	0.00	H
ATOM	2871	2HZ	LYS	300	16.117	21.256	47.129	1.00	0.00	H
ATOM	2872	3HZ	LYS	300	14.443	21.190	46.983	1.00	0.00	H
ATOM	2873	N	GLY	301	12.461	20.372	45.778	1.00	0.00	N
ATOM	2874	CA	GLY	301	11.731	21.382	46.474	1.00	0.00	C
ATOM	2875	C	GLY	301	12.122	22.678	45.854	1.00	0.00	C
ATOM	2876	O	GLY	301	12.740	22.704	44.791	1.00	0.00	O
ATOM	2877	H	GLY	301	13.477	20.290	45.922	1.00	0.00	H
ATOM	2878	1HA	GLY	301	12.033	21.310	47.518	1.00	0.00	H
ATOM	2879	2HA	GLY	301	10.676	21.149	46.327	1.00	0.00	H
ATOM	2880	N	ILE	302	11.773	23.795	46.516	1.00	0.00	N
ATOM	2881	CA	ILE	302	12.113	25.074	45.979	1.00	0.00	C
ATOM	2882	C	ILE	302	13.590	25.101	45.795	1.00	0.00	C
ATOM	2883	O	ILE	302	14.361	24.917	46.735	1.00	0.00	O
ATOM	2884	CB	ILE	302	11.700	26.223	46.852	1.00	0.00	C
ATOM	2885	CG1	ILE	302	12.017	27.565	46.171	1.00	0.00	C
ATOM	2886	CG2	ILE	302	12.347	26.031	48.230	1.00	0.00	C
ATOM	2887	CD1	ILE	302	11.371	28.767	46.859	1.00	0.00	C
ATOM	2888	H	ILE	302	11.261	23.728	47.407	1.00	0.00	H
ATOM	2889	HA	ILE	302	11.590	25.177	45.028	1.00	0.00	H
ATOM	2890	HB	ILE	302	10.612	26.215	46.930	1.00	0.00	H
ATOM	2891	1HG1	ILE	302	11.682	27.617	45.134	1.00	0.00	H
ATOM	2892	2HG1	ILE	302	13.081	27.795	46.137	1.00	0.00	H
ATOM	2893	1HG2	ILE	302	12.939	25.116	48.229	1.00	0.00	H
ATOM	2894	2HG2	ILE	302	12.992	26.881	48.450	1.00	0.00	H
ATOM	2895	3HG2	ILE	302	11.569	25.959	48.990	1.00	0.00	H
ATOM	2896	1HD1	ILE	302	10.796	28.427	47.721	1.00	0.00	H
ATOM	2897	2HD1	ILE	302	12.147	29.457	47.189	1.00	0.00	H
ATOM	2898	3HD1	ILE	302	10.708	29.274	46.158	1.00	0.00	H
ATOM	2899	N	LEU	303	14.007	25.313	44.536	1.00	0.00	N
ATOM	2900	CA	LEU	303	15.389	25.330	44.179	1.00	0.00	C
ATOM	2901	C	LEU	303	16.008	26.457	44.925	1.00	0.00	C
ATOM	2902	O	LEU	303	17.130	26.353	45.418	1.00	0.00	O
ATOM	2903	CB	LEU	303	15.605	25.636	42.686	1.00	0.00	C
ATOM	2904	CG	LEU	303	14.969	24.617	41.721	1.00	0.00	C
ATOM	2905	CD1	LEU	303	15.618	23.232	41.852	1.00	0.00	C
ATOM	2906	CD2	LEU	303	13.439	24.583	41.865	1.00	0.00	C
ATOM	2907	H	LEU	303	13.303	25.469	43.800	1.00	0.00	H
ATOM	2908	HA	LEU	303	15.800	24.365	44.476	1.00	0.00	H
ATOM	2909	1HB	LEU	303	16.677	25.646	42.492	1.00	0.00	H
ATOM	2910	2HB	LEU	303	15.165	26.610	42.471	1.00	0.00	H
ATOM	2911	HG	LEU	303	15.076	24.926	40.681	1.00	0.00	H
ATOM	2912	1HD1	LEU	303	16.400	23.267	42.610	1.00	0.00	H
ATOM	2913	2HD1	LEU	303	14.862	22.502	42.143	1.00	0.00	H
ATOM	2914	3HD1	LEU	303	16.052	22.941	40.895	1.00	0.00	H
ATOM	2915	1HD2	LEU	303	13.129	25.296	42.628	1.00	0.00	H
ATOM	2916	2HD2	LEU	303	12.978	24.847	40.913	1.00	0.00	H
ATOM	2917	3HD2	LEU	303	13.123	23.581	42.155	1.00	0.00	H
ATOM	2918	N	LYS	304	15.262	27.569	45.034	1.00	0.00	N
ATOM	2919	CA	LYS	304	15.783	28.750	45.650	1.00	0.00	C

ATOM	2920	C	LYS	304	16.148	28.473	47.072	1.00	0.00	C
ATOM	2921	O	LYS	304	17.219	28.875	47.520	1.00	0.00	O
ATOM	2922	CB	LYS	304	14.786	29.922	45.653	1.00	0.00	C
ATOM	2923	CG	LYS	304	14.564	30.544	44.272	1.00	0.00	C
ATOM	2924	CD	LYS	304	13.849	29.625	43.280	1.00	0.00	C
ATOM	2925	CE	LYS	304	13.634	30.266	41.907	1.00	0.00	C
ATOM	2926	NZ	LYS	304	12.942	29.318	41.007	1.00	0.00	N
ATOM	2927	H	LYS	304	14.299	27.571	44.668	1.00	0.00	H
ATOM	2928	HA	LYS	304	16.673	29.090	45.120	1.00	0.00	H
ATOM	2929	1HB	LYS	304	15.088	30.752	46.290	1.00	0.00	H
ATOM	2930	2HB	LYS	304	13.790	29.648	46.001	1.00	0.00	H
ATOM	2931	1HG	LYS	304	15.536	30.796	43.849	1.00	0.00	H
ATOM	2932	2HG	LYS	304	13.954	31.439	44.393	1.00	0.00	H
ATOM	2933	1HD	LYS	304	12.857	29.317	43.613	1.00	0.00	H
ATOM	2934	2HD	LYS	304	14.388	28.698	43.084	1.00	0.00	H
ATOM	2935	1HE	LYS	304	14.593	30.534	41.465	1.00	0.00	H
ATOM	2936	2HE	LYS	304	13.026	31.165	42.005	1.00	0.00	H
ATOM	2937	1HZ	LYS	304	12.760	28.437	41.509	1.00	0.00	H
ATOM	2938	2HZ	LYS	304	12.048	29.727	40.698	1.00	0.00	H
ATOM	2939	3HZ	LYS	304	13.534	29.128	40.186	1.00	0.00	H
ATOM	2940	N	ASP	305	15.287	27.767	47.827	1.00	0.00	N
ATOM	2941	CA	ASP	305	15.607	27.592	49.215	1.00	0.00	C
ATOM	2942	C	ASP	305	16.862	26.797	49.367	1.00	0.00	C
ATOM	2943	O	ASP	305	17.726	27.159	50.165	1.00	0.00	O
ATOM	2944	CB	ASP	305	14.513	26.886	50.034	1.00	0.00	C
ATOM	2945	CG	ASP	305	13.392	27.890	50.267	1.00	0.00	C
ATOM	2946	OD1	ASP	305	13.596	29.090	49.942	1.00	0.00	O
ATOM	2947	OD2	ASP	305	12.319	27.471	50.778	1.00	0.00	O
ATOM	2948	H	ASP	305	14.428	27.366	47.423	1.00	0.00	H
ATOM	2949	HA	ASP	305	15.751	28.558	49.698	1.00	0.00	H
ATOM	2950	1HB	ASP	305	14.960	26.567	50.975	1.00	0.00	H
ATOM	2951	2HB	ASP	305	14.164	26.032	49.452	1.00	0.00	H
ATOM	2952	N	LYS	306	17.018	25.697	48.606	1.00	0.00	N
ATOM	2953	CA	LYS	306	18.190	24.902	48.824	1.00	0.00	C
ATOM	2954	C	LYS	306	19.398	25.699	48.455	1.00	0.00	C
ATOM	2955	O	LYS	306	20.406	25.684	49.158	1.00	0.00	O
ATOM	2956	CB	LYS	306	18.210	23.580	48.037	1.00	0.00	C
ATOM	2957	CG	LYS	306	18.354	23.727	46.523	1.00	0.00	C
ATOM	2958	CD	LYS	306	18.700	22.400	45.844	1.00	0.00	C
ATOM	2959	CE	LYS	306	18.844	22.501	44.327	1.00	0.00	C
ATOM	2960	NZ	LYS	306	19.175	21.174	43.761	1.00	0.00	N
ATOM	2961	H	LYS	306	16.320	25.436	47.893	1.00	0.00	H
ATOM	2962	HA	LYS	306	18.240	24.620	49.875	1.00	0.00	H
ATOM	2963	1HB	LYS	306	17.270	23.060	48.225	1.00	0.00	H
ATOM	2964	2HB	LYS	306	19.056	22.990	48.388	1.00	0.00	H
ATOM	2965	1HG	LYS	306	19.140	24.431	46.250	1.00	0.00	H
ATOM	2966	2HG	LYS	306	17.437	24.087	46.055	1.00	0.00	H
ATOM	2967	1HD	LYS	306	17.903	21.686	46.056	1.00	0.00	H
ATOM	2968	2HD	LYS	306	19.648	22.044	46.246	1.00	0.00	H
ATOM	2969	1HE	LYS	306	19.639	23.202	44.074	1.00	0.00	H
ATOM	2970	2HE	LYS	306	17.910	22.850	43.886	1.00	0.00	H
ATOM	2971	1HZ	LYS	306	19.233	20.481	44.520	1.00	0.00	H
ATOM	2972	2HZ	LYS	306	18.441	20.891	43.095	1.00	0.00	H
ATOM	2973	3HZ	LYS	306	20.080	21.224	43.272	1.00	0.00	H
ATOM	2974	N	LYS	307	19.311	26.450	47.347	1.00	0.00	N
ATOM	2975	CA	LYS	307	20.430	27.216	46.887	1.00	0.00	C
ATOM	2976	C	LYS	307	20.794	28.205	47.945	1.00	0.00	C
ATOM	2977	O	LYS	307	21.972	28.465	48.185	1.00	0.00	O
ATOM	2978	CB	LYS	307	20.118	27.988	45.591	1.00	0.00	C
ATOM	2979	CG	LYS	307	21.337	28.616	44.908	1.00	0.00	C
ATOM	2980	CD	LYS	307	22.037	29.699	45.732	1.00	0.00	C
ATOM	2981	CE	LYS	307	23.252	30.313	45.035	1.00	0.00	C
ATOM	2982	NZ	LYS	307	23.851	31.358	45.895	1.00	0.00	N
ATOM	2983	H	LYS	307	18.426	26.476	46.819	1.00	0.00	H
ATOM	2984	HA	LYS	307	21.261	26.535	46.699	1.00	0.00	H
ATOM	2985	1HB	LYS	307	19.426	28.795	45.834	1.00	0.00	H
ATOM	2986	2HB	LYS	307	19.666	27.293	44.882	1.00	0.00	H
ATOM	2987	1HG	LYS	307	21.007	29.072	43.974	1.00	0.00	H

ATOM	2988	2HG	LYS	307	22.064	27.827	44.714	1.00	0.00	H
ATOM	2989	1HD	LYS	307	22.413	29.344	46.691	1.00	0.00	H
ATOM	2990	2HD	LYS	307	21.396	30.546	45.977	1.00	0.00	H
ATOM	2991	1HE	LYS	307	22.949	30.761	44.088	1.00	0.00	H
ATOM	2992	2HE	LYS	307	23.997	29.541	44.841	1.00	0.00	H
ATOM	2993	1HZ	LYS	307	23.312	31.434	46.769	1.00	0.00	H
ATOM	2994	2HZ	LYS	307	24.825	31.106	46.113	1.00	0.00	H
ATOM	2995	3HZ	LYS	307	23.832	32.261	45.401	1.00	0.00	H
ATOM	2996	N	ASN	308	19.788	28.784	48.622	1.00	0.00	N
ATOM	2997	CA	ASN	308	20.100	29.798	49.585	1.00	0.00	C
ATOM	2998	C	ASN	308	21.006	29.231	50.635	1.00	0.00	C
ATOM	2999	O	ASN	308	22.071	29.785	50.906	1.00	0.00	O
ATOM	3000	CB	ASN	308	18.848	30.327	50.307	1.00	0.00	C
ATOM	3001	CG	ASN	308	19.247	31.528	51.153	1.00	0.00	C
ATOM	3002	OD1	ASN	308	20.366	32.029	51.054	1.00	0.00	O
ATOM	3003	ND2	ASN	308	18.309	32.003	52.016	1.00	0.00	N
ATOM	3004	H	ASN	308	18.811	28.504	48.451	1.00	0.00	H
ATOM	3005	HA	ASN	308	20.597	30.631	49.089	1.00	0.00	H
ATOM	3006	1HB	ASN	308	18.450	29.533	50.939	1.00	0.00	H
ATOM	3007	2HB	ASN	308	18.112	30.618	49.557	1.00	0.00	H
ATOM	3008	1HD2	ASN	308	18.524	32.811	52.617	1.00	0.00	H
ATOM	3009	2HD2	ASN	308	17.383	31.554	52.068	1.00	0.00	H
ATOM	3010	N	ASP	309	20.605	28.106	51.258	1.00	0.00	N
ATOM	3011	CA	ASP	309	21.388	27.540	52.320	1.00	0.00	C
ATOM	3012	C	ASP	309	22.665	26.942	51.803	1.00	0.00	C
ATOM	3013	O	ASP	309	23.747	27.246	52.304	1.00	0.00	O
ATOM	3014	CB	ASP	309	20.635	26.430	53.073	1.00	0.00	C
ATOM	3015	CG	ASP	309	19.471	27.076	53.813	1.00	0.00	C
ATOM	3016	OD1	ASP	309	19.395	28.333	53.812	1.00	0.00	O
ATOM	3017	OD2	ASP	309	18.644	26.320	54.390	1.00	0.00	O
ATOM	3018	H	ASP	309	19.728	27.647	50.969	1.00	0.00	H
ATOM	3019	HA	ASP	309	21.657	28.292	53.061	1.00	0.00	H
ATOM	3020	1HB	ASP	309	21.333	25.966	53.769	1.00	0.00	H
ATOM	3021	2HB	ASP	309	20.279	25.709	52.336	1.00	0.00	H
ATOM	3022	N	ILE	310	22.562	26.078	50.772	1.00	0.00	N
ATOM	3023	CA	ILE	310	23.688	25.341	50.263	1.00	0.00	C
ATOM	3024	C	ILE	310	24.679	26.236	49.592	1.00	0.00	C
ATOM	3025	O	ILE	310	25.879	26.087	49.814	1.00	0.00	O
ATOM	3026	CB	ILE	310	23.289	24.288	49.273	1.00	0.00	C
ATOM	3027	CG1	ILE	310	22.391	23.238	49.948	1.00	0.00	C
ATOM	3028	CG2	ILE	310	24.575	23.700	48.668	1.00	0.00	C
ATOM	3029	CD1	ILE	310	23.080	22.501	51.096	1.00	0.00	C
ATOM	3030	H	ILE	310	21.641	25.940	50.331	1.00	0.00	H
ATOM	3031	HA	ILE	310	24.218	24.814	51.056	1.00	0.00	H
ATOM	3032	HB	ILE	310	22.677	24.765	48.507	1.00	0.00	H
ATOM	3033	1HG1	ILE	310	22.051	22.458	49.266	1.00	0.00	H
ATOM	3034	2HG1	ILE	310	21.483	23.659	50.379	1.00	0.00	H
ATOM	3035	1HG2	ILE	310	25.442	24.192	49.107	1.00	0.00	H
ATOM	3036	2HG2	ILE	310	24.620	22.631	48.877	1.00	0.00	H
ATOM	3037	3HG2	ILE	310	24.575	23.858	47.589	1.00	0.00	H
ATOM	3038	1HD1	ILE	310	24.097	22.876	51.210	1.00	0.00	H
ATOM	3039	2HD1	ILE	310	22.525	22.667	52.019	1.00	0.00	H
ATOM	3040	3HD1	ILE	310	23.109	21.433	50.877	1.00	0.00	H
ATOM	3041	N	GLU	311	24.186	27.194	48.779	1.00	0.00	N
ATOM	3042	CA	GLU	311	24.943	28.128	47.983	1.00	0.00	C
ATOM	3043	C	GLU	311	25.034	27.561	46.604	1.00	0.00	C
ATOM	3044	O	GLU	311	25.245	28.291	45.636	1.00	0.00	O
ATOM	3045	CB	GLU	311	26.400	28.389	48.424	1.00	0.00	C
ATOM	3046	CG	GLU	311	27.404	27.341	47.930	1.00	0.00	C
ATOM	3047	CD	GLU	311	28.788	27.726	48.434	1.00	0.00	C
ATOM	3048	OE1	GLU	311	28.894	28.759	49.148	1.00	0.00	O
ATOM	3049	OE2	GLU	311	29.759	26.993	48.108	1.00	0.00	O
ATOM	3050	H	GLU	311	23.160	27.265	48.721	1.00	0.00	H
ATOM	3051	HA	GLU	311	24.401	29.073	47.993	1.00	0.00	H
ATOM	3052	1HB	GLU	311	26.432	28.391	49.513	1.00	0.00	H
ATOM	3053	2HB	GLU	311	26.709	29.356	48.028	1.00	0.00	H
ATOM	3054	1HG	GLU	311	27.383	27.331	46.840	1.00	0.00	H
ATOM	3055	2HG	GLU	311	27.110	26.369	48.326	1.00	0.00	H

ATOM	3056	N	ALA	312	24.867	26.231	46.477	1.00	0.00	N
ATOM	3057	CA	ALA	312	24.906	25.633	45.176	1.00	0.00	C
ATOM	3058	C	ALA	312	23.634	24.875	45.010	1.00	0.00	C
ATOM	3059	O	ALA	312	23.143	24.248	45.948	1.00	0.00	O
ATOM	3060	CB	ALA	312	26.064	24.640	44.983	1.00	0.00	C
ATOM	3061	H	ALA	312	24.712	25.646	47.311	1.00	0.00	H
ATOM	3062	HA	ALA	312	24.991	26.446	44.456	1.00	0.00	H
ATOM	3063	1HB	ALA	312	26.649	24.580	45.900	1.00	0.00	H
ATOM	3064	2HB	ALA	312	25.662	23.655	44.744	1.00	0.00	H
ATOM	3065	3HB	ALA	312	26.702	24.979	44.166	1.00	0.00	H
ATOM	3066	N	GLN	313	23.033	24.961	43.810	1.00	0.00	N
ATOM	3067	CA	GLN	313	21.840	24.209	43.578	1.00	0.00	C
ATOM	3068	C	GLN	313	22.262	22.783	43.604	1.00	0.00	C
ATOM	3069	O	GLN	313	21.709	21.961	44.335	1.00	0.00	O
ATOM	3070	CB	GLN	313	21.222	24.531	42.204	1.00	0.00	C
ATOM	3071	CG	GLN	313	19.914	23.796	41.908	1.00	0.00	C
ATOM	3072	CD	GLN	313	19.409	24.248	40.546	1.00	0.00	C
ATOM	3073	OE1	GLN	313	20.146	24.834	39.754	1.00	0.00	O
ATOM	3074	NE2	GLN	313	18.107	23.967	40.266	1.00	0.00	N
ATOM	3075	H	GLN	313	23.426	25.559	43.069	1.00	0.00	H
ATOM	3076	HA	GLN	313	21.168	24.474	44.394	1.00	0.00	H
ATOM	3077	1HB	GLN	313	21.939	24.249	41.433	1.00	0.00	H
ATOM	3078	2HB	GLN	313	21.014	25.600	42.165	1.00	0.00	H
ATOM	3079	1HG	GLN	313	19.194	24.049	42.686	1.00	0.00	H
ATOM	3080	2HG	GLN	313	20.115	22.724	41.906	1.00	0.00	H
ATOM	3081	1HE2	GLN	313	17.702	24.247	39.361	1.00	0.00	H
ATOM	3082	2HE2	GLN	313	17.526	23.474	40.959	1.00	0.00	H
ATOM	3083	N	TRP	314	23.311	22.485	42.818	1.00	0.00	N
ATOM	3084	CA	TRP	314	23.881	21.180	42.738	1.00	0.00	C
ATOM	3085	C	TRP	314	25.260	21.370	43.255	1.00	0.00	C
ATOM	3086	O	TRP	314	26.227	21.379	42.499	1.00	0.00	O
ATOM	3087	CB	TRP	314	23.999	20.710	41.282	1.00	0.00	C
ATOM	3088	CG	TRP	314	22.655	20.632	40.606	1.00	0.00	C
ATOM	3089	CD1	TRP	314	21.909	21.637	40.066	1.00	0.00	C
ATOM	3090	CD2	TRP	314	21.902	19.424	40.433	1.00	0.00	C
ATOM	3091	NE1	TRP	314	20.730	21.131	39.578	1.00	0.00	N
ATOM	3092	CE2	TRP	314	20.714	19.769	39.793	1.00	0.00	C
ATOM	3093	CE3	TRP	314	22.179	18.135	40.779	1.00	0.00	C
ATOM	3094	CZ2	TRP	314	19.777	18.824	39.487	1.00	0.00	C
ATOM	3095	CZ3	TRP	314	21.234	17.182	40.471	1.00	0.00	C
ATOM	3096	CH2	TRP	314	20.057	17.522	39.839	1.00	0.00	C
ATOM	3097	H	TRP	314	23.723	23.235	42.245	1.00	0.00	H
ATOM	3098	HA	TRP	314	23.317	20.470	43.343	1.00	0.00	H
ATOM	3099	1HB	TRP	314	24.448	19.719	41.209	1.00	0.00	H
ATOM	3100	2HB	TRP	314	24.615	21.383	40.686	1.00	0.00	H
ATOM	3101	HD1	TRP	314	22.204	22.685	40.027	1.00	0.00	H
ATOM	3102	HE1	TRP	314	19.982	21.677	39.126	1.00	0.00	H
ATOM	3103	HE3	TRP	314	23.110	17.869	41.279	1.00	0.00	H
ATOM	3104	HZ2	TRP	314	18.846	19.088	38.985	1.00	0.00	H
ATOM	3105	HZ3	TRP	314	21.419	16.140	40.731	1.00	0.00	H
ATOM	3106	HH2	TRP	314	19.330	16.741	39.612	1.00	0.00	H
ATOM	3107	N	HIS	315	25.394	21.550	44.575	1.00	0.00	N
ATOM	3108	CA	HIS	315	26.710	21.750	45.084	1.00	0.00	C
ATOM	3109	C	HIS	315	27.413	20.459	44.874	1.00	0.00	C
ATOM	3110	O	HIS	315	28.636	20.413	44.749	1.00	0.00	O
ATOM	3111	CB	HIS	315	26.750	22.063	46.589	1.00	0.00	C
ATOM	3112	CG	HIS	315	28.077	22.611	47.025	1.00	0.00	C
ATOM	3113	ND1	HIS	315	29.203	21.848	47.241	1.00	0.00	N
ATOM	3114	CD2	HIS	315	28.448	23.898	47.276	1.00	0.00	C
ATOM	3115	CE1	HIS	315	30.191	22.703	47.607	1.00	0.00	C
ATOM	3116	NE2	HIS	315	29.780	23.959	47.642	1.00	0.00	N
ATOM	3117	H	HIS	315	24.575	21.544	45.200	1.00	0.00	H
ATOM	3118	HA	HIS	315	27.126	22.567	44.495	1.00	0.00	H
ATOM	3119	1HB	HIS	315	26.565	21.181	47.202	1.00	0.00	H
ATOM	3120	2HB	HIS	315	26.002	22.800	46.880	1.00	0.00	H
ATOM	3121	HD1	HIS	315	29.280	20.825	47.143	1.00	0.00	H
ATOM	3122	HD2	HIS	315	27.786	24.760	47.198	1.00	0.00	H
ATOM	3123	HE1	HIS	315	31.207	22.390	47.845	1.00	0.00	H

ATOM	3124	HE2	HIS	315	30.328	24.795	47.887	1.00	0.00	H
ATOM	3125	N	ASP	316	26.632	19.363	44.820	1.00	0.00	N
ATOM	3126	CA	ASP	316	27.255	18.084	44.726	1.00	0.00	C
ATOM	3127	C	ASP	316	27.668	17.819	43.324	1.00	0.00	C
ATOM	3128	O	ASP	316	27.269	16.820	42.727	1.00	0.00	O
ATOM	3129	CB	ASP	316	26.354	16.932	45.193	1.00	0.00	C
ATOM	3130	CG	ASP	316	26.248	17.068	46.702	1.00	0.00	C
ATOM	3131	OD1	ASP	316	26.964	17.944	47.256	1.00	0.00	O
ATOM	3132	OD2	ASP	316	25.459	16.310	47.324	1.00	0.00	O
ATOM	3133	H	ASP	316	25.605	19.447	44.846	1.00	0.00	H
ATOM	3134	HA	ASP	316	28.137	18.049	45.365	1.00	0.00	H
ATOM	3135	1HB	ASP	316	26.856	16.014	44.887	1.00	0.00	H
ATOM	3136	2HB	ASP	316	25.397	17.075	44.689	1.00	0.00	H
ATOM	3137	N	GLU	317	28.494	18.714	42.758	1.00	0.00	N
ATOM	3138	CA	GLU	317	29.027	18.404	41.475	1.00	0.00	C
ATOM	3139	C	GLU	317	29.978	17.306	41.754	1.00	0.00	C
ATOM	3140	O	GLU	317	30.193	16.472	40.869	1.00	0.00	O
ATOM	3141	CB	GLU	317	29.769	19.557	40.766	1.00	0.00	C
ATOM	3142	CG	GLU	317	31.038	20.061	41.451	1.00	0.00	C
ATOM	3143	CD	GLU	317	31.668	21.086	40.513	1.00	0.00	C
ATOM	3144	OE1	GLU	317	32.161	20.672	39.430	1.00	0.00	O
ATOM	3145	OE2	GLU	317	31.658	22.296	40.865	1.00	0.00	O
ATOM	3146	H	GLU	317	28.733	19.594	43.235	1.00	0.00	H
ATOM	3147	HA	GLU	317	28.239	18.091	40.789	1.00	0.00	H
ATOM	3148	1HB	GLU	317	29.085	20.403	40.699	1.00	0.00	H
ATOM	3149	2HB	GLU	317	30.058	19.208	39.774	1.00	0.00	H
ATOM	3150	1HG	GLU	317	31.681	19.193	41.599	1.00	0.00	H
ATOM	3151	2HG	GLU	317	30.729	20.507	42.396	1.00	0.00	H
ATOM	3152	N	SER	318	30.507	17.340	43.021	1.00	0.00	N
ATOM	3153	CA	SER	318	31.471	16.482	43.681	1.00	0.00	C
ATOM	3154	C	SER	318	31.683	15.359	42.781	1.00	0.00	C
ATOM	3155	O	SER	318	31.131	14.271	42.940	1.00	0.00	O
ATOM	3156	CB	SER	318	30.999	15.951	45.046	1.00	0.00	C
ATOM	3157	OG	SER	318	30.898	17.022	45.973	1.00	0.00	O
ATOM	3158	H	SER	318	30.156	18.112	43.605	1.00	0.00	H
ATOM	3159	HA	SER	318	32.365	17.090	43.817	1.00	0.00	H
ATOM	3160	1HB	SER	318	31.711	15.218	45.425	1.00	0.00	H
ATOM	3161	2HB	SER	318	30.022	15.477	44.942	1.00	0.00	H
ATOM	3162	HG	SER	318	31.605	17.736	45.751	1.00	0.00	H
ATOM	3163	N	HIS	319	32.511	15.687	41.781	1.00	0.00	N
ATOM	3164	CA	HIS	319	32.640	14.944	40.586	1.00	0.00	C
ATOM	3165	C	HIS	319	32.692	13.484	40.840	1.00	0.00	C
ATOM	3166	O	HIS	319	31.715	12.770	40.611	1.00	0.00	O
ATOM	3167	CB	HIS	319	33.869	15.405	39.763	1.00	0.00	C
ATOM	3168	CG	HIS	319	34.885	16.229	40.506	1.00	0.00	C
ATOM	3169	ND1	HIS	319	35.774	15.739	41.436	1.00	0.00	N
ATOM	3170	CD2	HIS	319	35.149	17.562	40.405	1.00	0.00	C
ATOM	3171	CE1	HIS	319	36.528	16.792	41.848	1.00	0.00	C
ATOM	3172	NE2	HIS	319	36.185	17.919	41.250	1.00	0.00	N
ATOM	3173	H	HIS	319	33.089	16.532	41.889	1.00	0.00	H
ATOM	3174	HA	HIS	319	31.806	15.114	39.905	1.00	0.00	H
ATOM	3175	1HB	HIS	319	33.507	16.013	38.933	1.00	0.00	H
ATOM	3176	2HB	HIS	319	34.382	14.514	39.399	1.00	0.00	H
ATOM	3177	HD1	HIS	319	35.852	14.763	41.757	1.00	0.00	H
ATOM	3178	HD2	HIS	319	34.617	18.251	39.749	1.00	0.00	H
ATOM	3179	HE1	HIS	319	37.325	16.715	42.587	1.00	0.00	H
ATOM	3180	HE2	HIS	319	36.596	18.853	41.383	1.00	0.00	H
ATOM	3181	N	LEU	320	33.829	13.006	41.338	1.00	0.00	N
ATOM	3182	CA	LEU	320	33.960	11.594	41.453	1.00	0.00	C
ATOM	3183	C	LEU	320	33.221	11.019	42.623	1.00	0.00	C
ATOM	3184	O	LEU	320	32.483	10.042	42.489	1.00	0.00	O
ATOM	3185	CB	LEU	320	35.438	11.190	41.608	1.00	0.00	C
ATOM	3186	CG	LEU	320	36.349	11.636	40.441	1.00	0.00	C
ATOM	3187	CD1	LEU	320	36.495	13.166	40.370	1.00	0.00	C
ATOM	3188	CD2	LEU	320	37.714	10.938	40.509	1.00	0.00	C
ATOM	3189	H	LEU	320	34.588	13.636	41.630	1.00	0.00	H
ATOM	3190	HA	LEU	320	33.586	11.051	40.584	1.00	0.00	H
ATOM	3191	1HB	LEU	320	35.490	10.103	41.670	1.00	0.00	H

ATOM	3192	2HB	LEU	320	35.823	11.646	42.519	1.00	0.00		H
ATOM	3193	HG	LEU	320	35.965	11.314	39.473	1.00	0.00		H
ATOM	3194	1HD1	LEU	320	35.915	13.624	41.171	1.00	0.00		H
ATOM	3195	2HD1	LEU	320	37.545	13.436	40.480	1.00	0.00		H
ATOM	3196	3HD1	LEU	320	36.128	13.522	39.407	1.00	0.00		H
ATOM	3197	1HD2	LEU	320	37.740	10.274	41.373	1.00	0.00		H
ATOM	3198	2HD2	LEU	320	37.870	10.356	39.600	1.00	0.00		H
ATOM	3199	3HD2	LEU	320	38.501	11.686	40.601	1.00	0.00		H
ATOM	3200	N	ASN	321	33.369	11.655	43.800	1.00	0.00		N
ATOM	3201	CA	ASN	321	32.981	11.026	45.032	1.00	0.00		C
ATOM	3202	C	ASN	321	31.507	10.933	45.227	1.00	0.00		C
ATOM	3203	O	ASN	321	30.830	11.938	45.420	1.00	0.00		O
ATOM	3204	CB	ASN	321	33.583	11.700	46.279	1.00	0.00		C
ATOM	3205	CG	ASN	321	33.564	10.699	47.429	1.00	0.00		C
ATOM	3206	OD1	ASN	321	34.621	10.221	47.835	1.00	0.00		O
ATOM	3207	ND2	ASN	321	32.356	10.377	47.969	1.00	0.00		N
ATOM	3208	H	ASN	321	33.765	12.605	43.817	1.00	0.00		H
ATOM	3209	HA	ASN	321	33.382	10.012	45.041	1.00	0.00		H
ATOM	3210	1HB	ASN	321	32.980	12.573	46.526	1.00	0.00		H
ATOM	3211	2HB	ASN	321	34.606	11.997	46.052	1.00	0.00		H
ATOM	3212	1HD2	ASN	321	32.303	9.707	48.750	1.00	0.00		H
ATOM	3213	2HD2	ASN	321	31.495	10.802	47.596	1.00	0.00		H
ATOM	3214	N	LYS	322	31.016	9.677	45.216	1.00	0.00		N
ATOM	3215	CA	LYS	322	29.662	9.267	45.453	1.00	0.00		C
ATOM	3216	C	LYS	322	29.164	8.606	44.218	1.00	0.00		C
ATOM	3217	O	LYS	322	29.905	7.895	43.539	1.00	0.00		O
ATOM	3218	CB	LYS	322	28.655	10.351	45.921	1.00	0.00		C
ATOM	3219	CG	LYS	322	28.204	11.408	44.904	1.00	0.00		C
ATOM	3220	CD	LYS	322	26.891	12.077	45.310	1.00	0.00		C
ATOM	3221	CE	LYS	322	26.960	12.783	46.661	1.00	0.00		C
ATOM	3222	NZ	LYS	322	27.034	14.246	46.472	1.00	0.00		N
ATOM	3223	H	LYS	322	31.691	8.925	45.014	1.00	0.00		H
ATOM	3224	HA	LYS	322	29.665	8.573	46.294	1.00	0.00		H
ATOM	3225	1HB	LYS	322	29.122	10.896	46.741	1.00	0.00		H
ATOM	3226	2HB	LYS	322	27.751	9.835	46.247	1.00	0.00		H
ATOM	3227	1HG	LYS	322	28.044	10.984	43.912	1.00	0.00		H
ATOM	3228	2HG	LYS	322	28.937	12.206	44.786	1.00	0.00		H
ATOM	3229	1HD	LYS	322	26.056	11.381	45.394	1.00	0.00		H
ATOM	3230	2HD	LYS	322	26.556	12.839	44.606	1.00	0.00		H
ATOM	3231	1HE	LYS	322	27.842	12.458	47.213	1.00	0.00		H
ATOM	3232	2HE	LYS	322	26.074	12.553	47.253	1.00	0.00		H
ATOM	3233	1HZ	LYS	322	27.022	14.463	45.465	1.00	0.00		H
ATOM	3234	2HZ	LYS	322	26.226	14.693	46.928	1.00	0.00		H
ATOM	3235	3HZ	LYS	322	27.905	14.603	46.890	1.00	0.00		H
ATOM	3236	N	TYR	323	27.877	8.812	43.892	1.00	0.00		N
ATOM	3237	CA	TYR	323	27.365	8.140	42.748	1.00	0.00		C
ATOM	3238	C	TYR	323	26.560	9.116	41.954	1.00	0.00		C
ATOM	3239	O	TYR	323	26.111	10.140	42.466	1.00	0.00		O
ATOM	3240	CB	TYR	323	26.425	6.999	43.149	1.00	0.00		C
ATOM	3241	CG	TYR	323	27.172	6.143	44.116	1.00	0.00		C
ATOM	3242	CD1	TYR	323	27.955	5.095	43.699	1.00	0.00		C
ATOM	3243	CD2	TYR	323	27.091	6.394	45.468	1.00	0.00		C
ATOM	3244	CE1	TYR	323	28.639	4.317	44.599	1.00	0.00		C
ATOM	3245	CE2	TYR	323	27.769	5.623	46.380	1.00	0.00		C
ATOM	3246	CZ	TYR	323	28.544	4.576	45.946	1.00	0.00		C
ATOM	3247	OH	TYR	323	29.242	3.783	46.876	1.00	0.00		O
ATOM	3248	H	TYR	323	27.280	9.436	44.452	1.00	0.00		H
ATOM	3249	HA	TYR	323	28.207	7.770	42.163	1.00	0.00		H
ATOM	3250	1HB	TYR	323	26.175	6.459	42.235	1.00	0.00		H
ATOM	3251	2HB	TYR	323	25.547	7.457	43.604	1.00	0.00		H
ATOM	3252	HD1	TYR	323	28.034	4.877	42.634	1.00	0.00		H
ATOM	3253	HD2	TYR	323	26.476	7.221	45.821	1.00	0.00		H
ATOM	3254	HE1	TYR	323	29.258	3.492	44.245	1.00	0.00		H
ATOM	3255	HE2	TYR	323	27.692	5.841	47.445	1.00	0.00		H
ATOM	3256	HH	TYR	323	28.865	3.948	47.820	1.00	0.00		H
ATOM	3257	N	PHE	324	26.404	8.832	40.650	1.00	0.00		N
ATOM	3258	CA	PHE	324	25.571	9.646	39.823	1.00	0.00		C
ATOM	3259	C	PHE	324	24.186	9.469	40.336	1.00	0.00		C

```
ATOM   3260  O   PHE   324      23.420  10.424  40.441  1.00  0.00           O
ATOM   3261  CB  PHE   324      25.516   9.189  38.347  1.00  0.00           C
ATOM   3262  CG  PHE   324      26.667   9.706  37.536  1.00  0.00           C
ATOM   3263  CD1 PHE   324      27.847   9.007  37.410  1.00  0.00           C
ATOM   3264  CD2 PHE   324      26.543  10.913  36.882  1.00  0.00           C
ATOM   3265  CE1 PHE   324      28.882   9.508  36.654  1.00  0.00           C
ATOM   3266  CE2 PHE   324      27.571  11.421  36.123  1.00  0.00           C
ATOM   3267  CZ  PHE   324      28.744  10.718  36.010  1.00  0.00           C
ATOM   3268  H   PHE   324      26.889   8.019  40.243  1.00  0.00           H
ATOM   3269  HA  PHE   324      25.936  10.666  39.940  1.00  0.00           H
ATOM   3270 1HB  PHE   324      24.613   9.523  37.835  1.00  0.00           H
ATOM   3271 2HB  PHE   324      25.536   8.104  38.240  1.00  0.00           H
ATOM   3272  HD1 PHE   324      27.962   8.047  37.914  1.00  0.00           H
ATOM   3273  HD2 PHE   324      25.613  11.475  36.968  1.00  0.00           H
ATOM   3274  HE1 PHE   324      29.812   8.946  36.564  1.00  0.00           H
ATOM   3275  HE2 PHE   324      27.454  12.377  35.613  1.00  0.00           H
ATOM   3276  HZ  PHE   324      29.564  11.115  35.412  1.00  0.00           H
ATOM   3277  N   LEU   325      23.861   8.213  40.695  1.00  0.00           N
ATOM   3278  CA  LEU   325      22.565   7.783  41.130  1.00  0.00           C
ATOM   3279  C   LEU   325      22.154   8.523  42.366  1.00  0.00           C
ATOM   3280  O   LEU   325      21.008   8.948  42.497  1.00  0.00           O
ATOM   3281  CB  LEU   325      22.578   6.295  41.501  1.00  0.00           C
ATOM   3282  CG  LEU   325      21.243   5.784  42.071  1.00  0.00           C
ATOM   3283  CD1 LEU   325      20.119   5.791  41.021  1.00  0.00           C
ATOM   3284  CD2 LEU   325      21.435   4.421  42.755  1.00  0.00           C
ATOM   3285  H   LEU   325      24.605   7.502  40.653  1.00  0.00           H
ATOM   3286  HA  LEU   325      21.821   7.967  40.354  1.00  0.00           H
ATOM   3287 1HB  LEU   325      23.346   6.135  42.257  1.00  0.00           H
ATOM   3288 2HB  LEU   325      22.800   5.718  40.603  1.00  0.00           H
ATOM   3289  HG  LEU   325      20.890   6.389  42.905  1.00  0.00           H
ATOM   3290 1HD1 LEU   325      20.508   6.163  40.073  1.00  0.00           H
ATOM   3291 2HD1 LEU   325      19.741   4.777  40.885  1.00  0.00           H
ATOM   3292 3HD1 LEU   325      19.309   6.437  41.359  1.00  0.00           H
ATOM   3293 1HD2 LEU   325      22.480   4.121  42.681  1.00  0.00           H
ATOM   3294 2HD2 LEU   325      21.152   4.497  43.804  1.00  0.00           H
ATOM   3295 3HD2 LEU   325      20.808   3.676  42.264  1.00  0.00           H
ATOM   3296  N   LEU   326      23.075   8.667  43.330  1.00  0.00           N
ATOM   3297  CA  LEU   326      22.749   9.347  44.548  1.00  0.00           C
ATOM   3298  C   LEU   326      22.616  10.799  44.259  1.00  0.00           C
ATOM   3299  O   LEU   326      21.899  11.523  44.946  1.00  0.00           O
ATOM   3300  CB  LEU   326      23.812   9.146  45.642  1.00  0.00           C
ATOM   3301  CG  LEU   326      23.773   7.738  46.252  1.00  0.00           C
ATOM   3302  CD1 LEU   326      22.500   7.562  47.098  1.00  0.00           C
ATOM   3303  CD2 LEU   326      23.909   6.638  45.177  1.00  0.00           C
ATOM   3304  H   LEU   326      24.022   8.286  43.193  1.00  0.00           H
ATOM   3305  HA  LEU   326      21.808   8.948  44.927  1.00  0.00           H
ATOM   3306 1HB  LEU   326      23.693   9.840  46.474  1.00  0.00           H
ATOM   3307 2HB  LEU   326      24.827   9.287  45.271  1.00  0.00           H
ATOM   3308  HG  LEU   326      24.642   7.580  46.889  1.00  0.00           H
ATOM   3309 1HD1 LEU   326      21.914   8.481  47.070  1.00  0.00           H
ATOM   3310 2HD1 LEU   326      21.906   6.741  46.695  1.00  0.00           H
ATOM   3311 3HD1 LEU   326      22.776   7.338  48.128  1.00  0.00           H
ATOM   3312 1HD2 LEU   326      24.005   7.099  44.194  1.00  0.00           H
ATOM   3313 2HD2 LEU   326      24.793   6.035  45.383  1.00  0.00           H
ATOM   3314 3HD2 LEU   326      23.024   6.001  45.193  1.00  0.00           H
ATOM   3315  N   ASN   327      23.303  11.267  43.211  1.00  0.00           N
ATOM   3316  CA  ASN   327      23.370  12.670  42.986  1.00  0.00           C
ATOM   3317  C   ASN   327      22.005  13.254  42.709  1.00  0.00           C
ATOM   3318  O   ASN   327      21.752  14.368  43.167  1.00  0.00           O
ATOM   3319  CB  ASN   327      24.390  13.029  41.895  1.00  0.00           C
ATOM   3320  CG  ASN   327      25.049  14.313  42.368  1.00  0.00           C
ATOM   3321  OD1 ASN   327      26.049  14.787  41.831  1.00  0.00           O
ATOM   3322  ND2 ASN   327      24.471  14.901  43.446  1.00  0.00           N
ATOM   3323  H   ASN   327      23.780  10.615  42.571  1.00  0.00           H
ATOM   3324  HA  ASN   327      23.777  13.195  43.849  1.00  0.00           H
ATOM   3325 1HB  ASN   327      23.805  13.155  40.983  1.00  0.00           H
ATOM   3326 2HB  ASN   327      25.076  12.183  41.852  1.00  0.00           H
ATOM   3327 1HD2 ASN   327      24.869  15.767  43.835  1.00  0.00           H
```

ATOM	3328	2HD2	ASN	327	23.633	14.481	43.874	1.00	0.00	H
ATOM	3329	N	LYS	328	21.089	12.555	41.978	1.00	0.00	N
ATOM	3330	CA	LYS	328	19.771	13.121	41.767	1.00	0.00	C
ATOM	3331	C	LYS	328	19.211	13.426	43.104	1.00	0.00	C
ATOM	3332	O	LYS	328	19.463	12.693	44.050	1.00	0.00	O
ATOM	3333	CB	LYS	328	18.750	12.263	40.983	1.00	0.00	C
ATOM	3334	CG	LYS	328	18.902	10.751	41.124	1.00	0.00	C
ATOM	3335	CD	LYS	328	20.036	10.188	40.268	1.00	0.00	C
ATOM	3336	CE	LYS	328	19.653	10.045	38.792	1.00	0.00	C
ATOM	3337	NZ	LYS	328	18.515	9.110	38.650	1.00	0.00	N
ATOM	3338	H	LYS	328	21.331	11.636	41.580	1.00	0.00	H
ATOM	3339	HA	LYS	328	19.902	14.022	41.168	1.00	0.00	H
ATOM	3340	1HB	LYS	328	18.857	12.498	39.924	1.00	0.00	H
ATOM	3341	2HB	LYS	328	17.752	12.519	41.340	1.00	0.00	H
ATOM	3342	1HG	LYS	328	18.004	10.207	40.828	1.00	0.00	H
ATOM	3343	2HG	LYS	328	19.116	10.442	42.147	1.00	0.00	H
ATOM	3344	1HD	LYS	328	20.358	9.197	40.589	1.00	0.00	H
ATOM	3345	2HD	LYS	328	20.929	10.812	40.285	1.00	0.00	H
ATOM	3346	1HE	LYS	328	20.498	9.659	38.221	1.00	0.00	H
ATOM	3347	2HE	LYS	328	19.365	11.013	38.384	1.00	0.00	H
ATOM	3348	1HZ	LYS	328	18.235	8.764	39.579	1.00	0.00	H
ATOM	3349	2HZ	LYS	328	17.720	9.599	38.213	1.00	0.00	H
ATOM	3350	3HZ	LYS	328	18.795	8.314	38.058	1.00	0.00	H
ATOM	3351	N	PRO	329	18.490	14.528	43.136	1.00	0.00	N
ATOM	3352	CA	PRO	329	17.995	15.142	44.344	1.00	0.00	C
ATOM	3353	C	PRO	329	17.563	14.144	45.354	1.00	0.00	C
ATOM	3354	O	PRO	329	16.396	13.757	45.352	1.00	0.00	O
ATOM	3355	CB	PRO	329	16.840	16.054	43.919	1.00	0.00	C
ATOM	3356	CG	PRO	329	16.999	16.206	42.397	1.00	0.00	C
ATOM	3357	CD	PRO	329	17.707	14.917	41.977	1.00	0.00	C
ATOM	3358	HA	PRO	329	18.743	15.765	44.832	1.00	0.00	H
ATOM	3359	1HB	PRO	329	16.999	16.980	44.471	1.00	0.00	H
ATOM	3360	2HB	PRO	329	15.938	15.517	44.214	1.00	0.00	H
ATOM	3361	1HG	PRO	329	17.591	17.088	42.153	1.00	0.00	H
ATOM	3362	2HG	PRO	329	16.028	16.308	41.911	1.00	0.00	H
ATOM	3363	1HD	PRO	329	17.028	14.081	41.804	1.00	0.00	H
ATOM	3364	2HD	PRO	329	18.437	15.058	41.180	1.00	0.00	H
ATOM	3365	N	THR	330	18.507	13.736	46.223	1.00	0.00	N
ATOM	3366	CA	THR	330	18.272	12.783	47.254	1.00	0.00	C
ATOM	3367	C	THR	330	19.467	12.850	48.135	1.00	0.00	C
ATOM	3368	O	THR	330	19.475	12.264	49.215	1.00	0.00	O
ATOM	3369	CB	THR	330	18.217	11.350	46.783	1.00	0.00	C
ATOM	3370	OG1	THR	330	19.439	10.996	46.151	1.00	0.00	O
ATOM	3371	CG2	THR	330	17.033	11.140	45.823	1.00	0.00	C
ATOM	3372	H	THR	330	19.452	14.135	46.137	1.00	0.00	H
ATOM	3373	HA	THR	330	17.356	13.108	47.747	1.00	0.00	H
ATOM	3374	HB	THR	330	18.096	10.672	47.628	1.00	0.00	H
ATOM	3375	HG1	THR	330	19.492	11.449	45.228	1.00	0.00	H
ATOM	3376	1HG2	THR	330	16.495	12.079	45.697	1.00	0.00	H
ATOM	3377	2HG2	THR	330	17.404	10.802	44.855	1.00	0.00	H
ATOM	3378	3HG2	THR	330	16.359	10.388	46.235	1.00	0.00	H
ATOM	3379	N	LYS	331	20.510	13.596	47.715	1.00	0.00	N
ATOM	3380	CA	LYS	331	21.658	13.604	48.564	1.00	0.00	C
ATOM	3381	C	LYS	331	21.219	14.380	49.761	1.00	0.00	C
ATOM	3382	O	LYS	331	20.372	15.265	49.651	1.00	0.00	O
ATOM	3383	CB	LYS	331	22.912	14.261	47.976	1.00	0.00	C
ATOM	3384	CG	LYS	331	24.225	13.648	48.472	1.00	0.00	C
ATOM	3385	CD	LYS	331	24.389	13.572	49.985	1.00	0.00	C
ATOM	3386	CE	LYS	331	25.663	12.842	50.413	1.00	0.00	C
ATOM	3387	NZ	LYS	331	25.531	12.388	51.815	1.00	0.00	N
ATOM	3388	H	LYS	331	20.479	14.128	46.833	1.00	0.00	H
ATOM	3389	HA	LYS	331	21.850	12.549	48.759	1.00	0.00	H
ATOM	3390	1HB	LYS	331	22.910	15.315	48.253	1.00	0.00	H
ATOM	3391	2HB	LYS	331	22.881	14.151	46.892	1.00	0.00	H
ATOM	3392	1HG	LYS	331	25.045	14.256	48.089	1.00	0.00	H
ATOM	3393	2HG	LYS	331	24.285	12.628	48.090	1.00	0.00	H
ATOM	3394	1HD	LYS	331	23.569	13.047	50.477	1.00	0.00	H
ATOM	3395	2HD	LYS	331	24.438	14.552	50.458	1.00	0.00	H

ATOM	3396	1HE	LYS	331	26.516	13.514	50.332	1.00	0.00	H
ATOM	3397	2HE	LYS	331	25.825	11.977	49.769	1.00	0.00	H
ATOM	3398	1HZ	LYS	331	24.610	12.668	52.181	1.00	0.00	H
ATOM	3399	2HZ	LYS	331	25.618	11.362	51.853	1.00	0.00	H
ATOM	3400	3HZ	LYS	331	26.272	12.817	52.386	1.00	0.00	H
ATOM	3401	N	ILE	332	21.784	14.062	50.939	1.00	0.00	N
ATOM	3402	CA	ILE	332	21.342	14.644	52.172	1.00	0.00	C
ATOM	3403	C	ILE	332	21.553	16.121	52.152	1.00	0.00	C
ATOM	3404	O	ILE	332	20.758	16.862	52.728	1.00	0.00	O
ATOM	3405	CB	ILE	332	22.072	14.114	53.379	1.00	0.00	C
ATOM	3406	CG1	ILE	332	23.561	14.495	53.330	1.00	0.00	C
ATOM	3407	CG2	ILE	332	21.826	12.596	53.459	1.00	0.00	C
ATOM	3408	CD1	ILE	332	24.290	14.284	54.658	1.00	0.00	C
ATOM	3409	H	ILE	332	22.556	13.380	50.955	1.00	0.00	H
ATOM	3410	HA	ILE	332	20.281	14.445	52.324	1.00	0.00	H
ATOM	3411	HB	ILE	332	21.677	14.617	54.261	1.00	0.00	H
ATOM	3412	1HG1	ILE	332	23.735	15.540	53.073	1.00	0.00	H
ATOM	3413	2HG1	ILE	332	24.132	13.924	52.598	1.00	0.00	H
ATOM	3414	1HG2	ILE	332	21.190	12.286	52.629	1.00	0.00	H
ATOM	3415	2HG2	ILE	332	22.778	12.069	53.402	1.00	0.00	H
ATOM	3416	3HG2	ILE	332	21.334	12.356	54.401	1.00	0.00	H
ATOM	3417	1HD1	ILE	332	23.591	13.894	55.398	1.00	0.00	H
ATOM	3418	2HD1	ILE	332	25.103	13.572	54.517	1.00	0.00	H
ATOM	3419	3HD1	ILE	332	24.694	15.234	55.005	1.00	0.00	H
ATOM	3420	N	LEU	333	22.615	16.605	51.481	1.00	0.00	N
ATOM	3421	CA	LEU	333	22.866	18.011	51.586	1.00	0.00	C
ATOM	3422	C	LEU	333	22.334	18.740	50.390	1.00	0.00	C
ATOM	3423	O	LEU	333	21.128	18.814	50.188	1.00	0.00	O
ATOM	3424	CB	LEU	333	24.348	18.375	51.772	1.00	0.00	C
ATOM	3425	CG	LEU	333	24.550	19.883	52.016	1.00	0.00	C
ATOM	3426	CD1	LEU	333	23.819	20.341	53.291	1.00	0.00	C
ATOM	3427	CD2	LEU	333	26.039	20.259	52.035	1.00	0.00	C
ATOM	3428	H	LEU	333	23.220	15.991	50.917	1.00	0.00	H
ATOM	3429	HA	LEU	333	22.388	18.426	52.473	1.00	0.00	H
ATOM	3430	1HB	LEU	333	24.947	18.116	50.899	1.00	0.00	H
ATOM	3431	2HB	LEU	333	24.794	17.858	52.621	1.00	0.00	H
ATOM	3432	HG	LEU	333	24.165	20.470	51.182	1.00	0.00	H
ATOM	3433	1HD1	LEU	333	23.313	19.489	53.746	1.00	0.00	H
ATOM	3434	2HD1	LEU	333	24.540	20.753	53.995	1.00	0.00	H
ATOM	3435	3HD1	LEU	333	23.084	21.104	53.034	1.00	0.00	H
ATOM	3436	1HD2	LEU	333	26.641	19.366	51.869	1.00	0.00	H
ATOM	3437	2HD2	LEU	333	26.241	20.984	51.247	1.00	0.00	H
ATOM	3438	3HD2	LEU	333	26.292	20.693	53.002	1.00	0.00	H
ATOM	3439	N	SER	334	23.227	19.303	49.556	1.00	0.00	N
ATOM	3440	CA	SER	334	22.815	20.174	48.490	1.00	0.00	C
ATOM	3441	C	SER	334	21.764	19.543	47.615	1.00	0.00	C
ATOM	3442	O	SER	334	20.758	20.197	47.345	1.00	0.00	O
ATOM	3443	CB	SER	334	23.992	20.643	47.610	1.00	0.00	C
ATOM	3444	OG	SER	334	23.529	21.501	46.579	1.00	0.00	O
ATOM	3445	H	SER	334	24.229	19.105	49.684	1.00	0.00	H
ATOM	3446	HA	SER	334	22.392	21.107	48.861	1.00	0.00	H
ATOM	3447	1HB	SER	334	24.488	19.788	47.151	1.00	0.00	H
ATOM	3448	2HB	SER	334	24.722	21.186	48.209	1.00	0.00	H
ATOM	3449	HG	SER	334	24.003	22.412	46.650	1.00	0.00	H
ATOM	3450	N	PRO	335	21.899	18.330	47.158	1.00	0.00	N
ATOM	3451	CA	PRO	335	20.859	17.820	46.305	1.00	0.00	C
ATOM	3452	C	PRO	335	19.605	17.492	47.041	1.00	0.00	C
ATOM	3453	O	PRO	335	18.686	16.997	46.388	1.00	0.00	O
ATOM	3454	CB	PRO	335	21.468	16.684	45.479	1.00	0.00	C
ATOM	3455	CG	PRO	335	22.905	16.541	46.006	1.00	0.00	C
ATOM	3456	CD	PRO	335	23.197	17.884	46.680	1.00	0.00	C
ATOM	3457	HA	PRO	335	20.564	18.519	45.523	1.00	0.00	H
ATOM	3458	1HB	PRO	335	21.412	17.029	44.446	1.00	0.00	H
ATOM	3459	2HB	PRO	335	20.837	15.819	45.686	1.00	0.00	H
ATOM	3460	1HG	PRO	335	23.502	16.352	45.113	1.00	0.00	H
ATOM	3461	2HG	PRO	335	22.857	15.698	46.695	1.00	0.00	H
ATOM	3462	1HD	PRO	335	23.801	17.809	47.583	1.00	0.00	H
ATOM	3463	2HD	PRO	335	23.512	18.670	45.994	1.00	0.00	H

ATOM	3464	N	GLU	336	19.575	17.755	48.372	1.00	0.00	N
ATOM	3465	CA	GLU	336	18.470	17.548	49.279	1.00	0.00	C
ATOM	3466	C	GLU	336	17.185	17.642	48.537	1.00	0.00	C
ATOM	3467	O	GLU	336	16.692	18.732	48.246	1.00	0.00	O
ATOM	3468	CB	GLU	336	18.418	18.586	50.418	1.00	0.00	C
ATOM	3469	CG	GLU	336	18.453	20.030	49.901	1.00	0.00	C
ATOM	3470	CD	GLU	336	18.762	20.971	51.059	1.00	0.00	C
ATOM	3471	OE1	GLU	336	18.934	20.470	52.202	1.00	0.00	O
ATOM	3472	OE2	GLU	336	18.828	22.206	50.814	1.00	0.00	O
ATOM	3473	H	GLU	336	20.435	18.145	48.780	1.00	0.00	H
ATOM	3474	HA	GLU	336	18.547	16.561	49.736	1.00	0.00	H
ATOM	3475	1HB	GLU	336	19.254	18.490	51.109	1.00	0.00	H
ATOM	3476	2HB	GLU	336	17.513	18.500	51.020	1.00	0.00	H
ATOM	3477	1HG	GLU	336	17.483	20.281	49.472	1.00	0.00	H
ATOM	3478	2HG	GLU	336	19.226	20.120	49.138	1.00	0.00	H
ATOM	3479	N	TYR	337	16.633	16.466	48.185	1.00	0.00	N
ATOM	3480	CA	TYR	337	15.420	16.433	47.432	1.00	0.00	C
ATOM	3481	C	TYR	337	14.430	17.194	48.240	1.00	0.00	C
ATOM	3482	O	TYR	337	13.956	18.250	47.828	1.00	0.00	O
ATOM	3483	CB	TYR	337	14.899	15.002	47.283	1.00	0.00	C
ATOM	3484	CG	TYR	337	13.666	15.028	46.458	1.00	0.00	C
ATOM	3485	CD1	TYR	337	12.443	15.315	47.015	1.00	0.00	C
ATOM	3486	CD2	TYR	337	13.746	14.753	45.113	1.00	0.00	C
ATOM	3487	CE1	TYR	337	11.311	15.328	46.234	1.00	0.00	C
ATOM	3488	CE2	TYR	337	12.621	14.762	44.327	1.00	0.00	C
ATOM	3489	CZ	TYR	337	11.402	15.050	44.891	1.00	0.00	C
ATOM	3490	OH	TYR	337	10.242	15.060	44.090	1.00	0.00	O
ATOM	3491	H	TYR	337	17.088	15.584	48.460	1.00	0.00	H
ATOM	3492	HA	TYR	337	15.654	16.910	46.480	1.00	0.00	H
ATOM	3493	1HB	TYR	337	14.680	14.604	48.274	1.00	0.00	H
ATOM	3494	2HB	TYR	337	15.665	14.399	46.795	1.00	0.00	H
ATOM	3495	HD1	TYR	337	12.369	15.533	48.080	1.00	0.00	H
ATOM	3496	HD2	TYR	337	14.713	14.525	44.666	1.00	0.00	H
ATOM	3497	HE1	TYR	337	10.343	15.558	46.679	1.00	0.00	H
ATOM	3498	HE2	TYR	337	12.694	14.542	43.262	1.00	0.00	H
ATOM	3499	HH	TYR	337	9.966	16.033	43.896	1.00	0.00	H
ATOM	3500	N	CYS	338	14.109	16.673	49.435	1.00	0.00	N
ATOM	3501	CA	CYS	338	13.277	17.399	50.342	1.00	0.00	C
ATOM	3502	C	CYS	338	13.989	17.315	51.643	1.00	0.00	C
ATOM	3503	O	CYS	338	13.386	17.395	52.712	1.00	0.00	O
ATOM	3504	CB	CYS	338	11.876	16.792	50.529	1.00	0.00	C
ATOM	3505	SG	CYS	338	10.811	17.035	49.076	1.00	0.00	S
ATOM	3506	H	CYS	338	14.464	15.743	49.699	1.00	0.00	H
ATOM	3507	HA	CYS	338	13.233	18.404	49.923	1.00	0.00	H
ATOM	3508	1HB	CYS	338	11.341	17.226	51.374	1.00	0.00	H
ATOM	3509	2HB	CYS	338	11.906	15.717	50.707	1.00	0.00	H
ATOM	3510	HG	CYS	338	10.717	18.343	48.803	1.00	0.00	H
ATOM	3511	N	TRP	339	15.323	17.158	51.567	1.00	0.00	N
ATOM	3512	CA	TRP	339	16.108	17.085	52.757	1.00	0.00	C
ATOM	3513	C	TRP	339	16.105	18.421	53.421	1.00	0.00	C
ATOM	3514	O	TRP	339	16.115	18.507	54.647	1.00	0.00	O
ATOM	3515	CB	TRP	339	17.569	16.664	52.521	1.00	0.00	C
ATOM	3516	CG	TRP	339	17.763	15.170	52.415	1.00	0.00	C
ATOM	3517	CD1	TRP	339	17.577	14.320	51.364	1.00	0.00	C
ATOM	3518	CD2	TRP	339	18.216	14.366	53.514	1.00	0.00	C
ATOM	3519	NE1	TRP	339	17.880	13.033	51.744	1.00	0.00	N
ATOM	3520	CE2	TRP	339	18.277	13.048	53.066	1.00	0.00	C
ATOM	3521	CE3	TRP	339	18.552	14.701	54.795	1.00	0.00	C
ATOM	3522	CZ2	TRP	339	18.678	12.039	53.897	1.00	0.00	C
ATOM	3523	CZ3	TRP	339	18.958	13.684	55.629	1.00	0.00	C
ATOM	3524	CH2	TRP	339	19.019	12.378	55.188	1.00	0.00	C
ATOM	3525	H	TRP	339	15.779	17.090	50.646	1.00	0.00	H
ATOM	3526	HA	TRP	339	15.674	16.337	53.421	1.00	0.00	H
ATOM	3527	1HB	TRP	339	18.250	16.978	53.311	1.00	0.00	H
ATOM	3528	2HB	TRP	339	18.000	17.067	51.604	1.00	0.00	H
ATOM	3529	HD1	TRP	339	17.238	14.616	50.371	1.00	0.00	H
ATOM	3530	HE1	TRP	339	17.820	12.198	51.143	1.00	0.00	H
ATOM	3531	HE3	TRP	339	18.500	15.732	55.142	1.00	0.00	H

ATOM	3532	HZ2	TRP	339	18.726	11.006	53.551	1.00	0.00	H
ATOM	3533	HZ3	TRP	339	19.236	13.914	56.657	1.00	0.00	H
ATOM	3534	HH2	TRP	339	19.344	11.597	55.876	1.00	0.00	H
ATOM	3535	N	ASP	340	16.084	19.507	52.626	1.00	0.00	N
ATOM	3536	CA	ASP	340	16.220	20.808	53.210	1.00	0.00	C
ATOM	3537	C	ASP	340	15.106	21.092	54.169	1.00	0.00	C
ATOM	3538	O	ASP	340	15.311	21.083	55.381	1.00	0.00	O
ATOM	3539	CB	ASP	340	16.200	21.927	52.156	1.00	0.00	C
ATOM	3540	CG	ASP	340	16.861	23.152	52.768	1.00	0.00	C
ATOM	3541	OD1	ASP	340	17.663	22.967	53.721	1.00	0.00	O
ATOM	3542	OD2	ASP	340	16.587	24.283	52.284	1.00	0.00	O
ATOM	3543	H	ASP	340	15.971	19.403	51.607	1.00	0.00	H
ATOM	3544	HA	ASP	340	17.158	20.899	53.757	1.00	0.00	H
ATOM	3545	1HB	ASP	340	15.158	22.127	51.903	1.00	0.00	H
ATOM	3546	2HB	ASP	340	16.754	21.574	51.286	1.00	0.00	H
ATOM	3547	N	TYR	341	13.880	21.325	53.655	1.00	0.00	N
ATOM	3548	CA	TYR	341	12.811	21.631	54.562	1.00	0.00	C
ATOM	3549	C	TYR	341	11.534	21.445	53.812	1.00	0.00	C
ATOM	3550	O	TYR	341	10.693	22.343	53.811	1.00	0.00	O
ATOM	3551	CB	TYR	341	12.732	23.114	54.977	1.00	0.00	C
ATOM	3552	CG	TYR	341	14.018	23.591	55.556	1.00	0.00	C
ATOM	3553	CD1	TYR	341	14.307	23.445	56.892	1.00	0.00	C
ATOM	3554	CD2	TYR	341	14.940	24.202	54.740	1.00	0.00	C
ATOM	3555	CE1	TYR	341	15.503	23.901	57.399	1.00	0.00	C
ATOM	3556	CE2	TYR	341	16.134	24.661	55.240	1.00	0.00	C
ATOM	3557	CZ	TYR	341	16.418	24.510	56.574	1.00	0.00	C
ATOM	3558	OH	TYR	341	17.643	24.979	57.094	1.00	0.00	O
ATOM	3559	H	TYR	341	13.716	21.284	52.638	1.00	0.00	H
ATOM	3560	HA	TYR	341	12.893	20.937	55.398	1.00	0.00	H
ATOM	3561	1HB	TYR	341	11.958	23.280	55.726	1.00	0.00	H
ATOM	3562	2HB	TYR	341	12.502	23.757	54.127	1.00	0.00	H
ATOM	3563	HD1	TYR	341	13.585	22.965	57.553	1.00	0.00	H
ATOM	3564	HD2	TYR	341	14.720	24.324	53.679	1.00	0.00	H
ATOM	3565	HE1	TYR	341	15.725	23.778	58.459	1.00	0.00	H
ATOM	3566	HE2	TYR	341	16.853	25.143	54.579	1.00	0.00	H
ATOM	3567	HH	TYR	341	18.264	25.250	56.318	1.00	0.00	H
ATOM	3568	N	HIS	342	11.324	20.291	53.157	1.00	0.00	N
ATOM	3569	CA	HIS	342	10.090	20.217	52.432	1.00	0.00	C
ATOM	3570	C	HIS	342	9.505	18.855	52.578	1.00	0.00	C
ATOM	3571	O	HIS	342	10.209	17.874	52.807	1.00	0.00	O
ATOM	3572	CB	HIS	342	10.247	20.457	50.920	1.00	0.00	C
ATOM	3573	CG	HIS	342	10.701	21.845	50.578	1.00	0.00	C
ATOM	3574	ND1	HIS	342	9.855	22.924	50.450	1.00	0.00	N
ATOM	3575	CD2	HIS	342	11.951	22.322	50.329	1.00	0.00	C
ATOM	3576	CE1	HIS	342	10.629	23.992	50.131	1.00	0.00	C
ATOM	3577	NE2	HIS	342	11.908	23.676	50.046	1.00	0.00	N
ATOM	3578	H	HIS	342	12.001	19.515	53.174	1.00	0.00	H
ATOM	3579	HA	HIS	342	9.389	20.954	52.824	1.00	0.00	H
ATOM	3580	1HB	HIS	342	9.323	20.313	50.358	1.00	0.00	H
ATOM	3581	2HB	HIS	342	10.973	19.795	50.447	1.00	0.00	H
ATOM	3582	HD1	HIS	342	8.832	22.921	50.572	1.00	0.00	H
ATOM	3583	HD2	HIS	342	12.860	21.720	50.349	1.00	0.00	H
ATOM	3584	HE1	HIS	342	10.239	24.996	49.964	1.00	0.00	H
ATOM	3585	HE2	HIS	342	12.697	24.298	49.819	1.00	0.00	H
ATOM	3586	N	ILE	343	8.165	18.783	52.464	1.00	0.00	N
ATOM	3587	CA	ILE	343	7.472	17.533	52.467	1.00	0.00	C
ATOM	3588	C	ILE	343	6.905	17.422	51.092	1.00	0.00	C
ATOM	3589	O	ILE	343	6.523	18.429	50.498	1.00	0.00	O
ATOM	3590	CB	ILE	343	6.331	17.470	53.441	1.00	0.00	C
ATOM	3591	CG1	ILE	343	5.808	16.029	53.559	1.00	0.00	C
ATOM	3592	CG2	ILE	343	5.269	18.490	52.999	1.00	0.00	C
ATOM	3593	CD1	ILE	343	6.816	15.065	54.185	1.00	0.00	C
ATOM	3594	H	ILE	343	7.623	19.654	52.371	1.00	0.00	H
ATOM	3595	HA	ILE	343	8.244	16.797	52.690	1.00	0.00	H
ATOM	3596	HB	ILE	343	6.716	17.716	54.430	1.00	0.00	H
ATOM	3597	1HG1	ILE	343	5.543	15.583	52.600	1.00	0.00	H
ATOM	3598	2HG1	ILE	343	4.910	15.941	54.171	1.00	0.00	H
ATOM	3599	1HG2	ILE	343	5.607	18.999	52.096	1.00	0.00	H

ATOM	3600	2HG2	ILE	343	4.331	17.973	52.794	1.00	0.00	H
ATOM	3601	3HG2	ILE	343	5.114	19.221	53.792	1.00	0.00	H
ATOM	3602	1HD1	ILE	343	7.730	15.604	54.430	1.00	0.00	H
ATOM	3603	2HD1	ILE	343	6.393	14.635	55.093	1.00	0.00	H
ATOM	3604	3HD1	ILE	343	7.043	14.267	53.478	1.00	0.00	H
ATOM	3605	N	GLY	344	6.844	16.203	50.527	1.00	0.00	N
ATOM	3606	CA	GLY	344	6.372	16.128	49.176	1.00	0.00	C
ATOM	3607	C	GLY	344	5.021	15.494	49.159	1.00	0.00	C
ATOM	3608	O	GLY	344	4.800	14.458	49.783	1.00	0.00	O
ATOM	3609	H	GLY	344	7.125	15.357	51.044	1.00	0.00	H
ATOM	3610	1HA	GLY	344	7.064	15.529	48.584	1.00	0.00	H
ATOM	3611	2HA	GLY	344	6.309	17.133	48.759	1.00	0.00	H
ATOM	3612	N	LEU	345	4.076	16.108	48.418	1.00	0.00	N
ATOM	3613	CA	LEU	345	2.764	15.541	48.315	1.00	0.00	C
ATOM	3614	C	LEU	345	2.718	14.786	47.024	1.00	0.00	C
ATOM	3615	O	LEU	345	3.242	15.217	45.998	1.00	0.00	O
ATOM	3616	CB	LEU	345	1.617	16.577	48.385	1.00	0.00	C
ATOM	3617	CG	LEU	345	1.585	17.639	47.268	1.00	0.00	C
ATOM	3618	CD1	LEU	345	1.188	17.040	45.911	1.00	0.00	C
ATOM	3619	CD2	LEU	345	0.699	18.832	47.661	1.00	0.00	C
ATOM	3620	H	LEU	345	4.297	16.985	47.925	1.00	0.00	H
ATOM	3621	HA	LEU	345	2.634	14.884	49.175	1.00	0.00	H
ATOM	3622	1HB	LEU	345	1.709	17.112	49.329	1.00	0.00	H
ATOM	3623	2HB	LEU	345	0.673	16.033	48.333	1.00	0.00	H
ATOM	3624	HG	LEU	345	2.554	18.116	47.127	1.00	0.00	H
ATOM	3625	1HD1	LEU	345	1.008	15.970	46.023	1.00	0.00	H
ATOM	3626	2HD1	LEU	345	0.280	17.524	45.551	1.00	0.00	H
ATOM	3627	3HD1	LEU	345	1.992	17.199	45.193	1.00	0.00	H
ATOM	3628	1HD2	LEU	345	0.282	18.664	48.654	1.00	0.00	H
ATOM	3629	2HD2	LEU	345	1.297	19.743	47.667	1.00	0.00	H
ATOM	3630	3HD2	LEU	345	-0.112	18.935	46.940	1.00	0.00	H
ATOM	3631	N	PRO	346	2.140	13.624	47.084	1.00	0.00	N
ATOM	3632	CA	PRO	346	2.120	12.778	45.921	1.00	0.00	C
ATOM	3633	C	PRO	346	1.045	13.032	44.913	1.00	0.00	C
ATOM	3634	O	PRO	346	-0.015	13.551	45.259	1.00	0.00	O
ATOM	3635	CB	PRO	346	2.103	11.337	46.440	1.00	0.00	C
ATOM	3636	CG	PRO	346	1.688	11.458	47.915	1.00	0.00	C
ATOM	3637	CD	PRO	346	2.191	12.852	48.314	1.00	0.00	C
ATOM	3638	HA	PRO	346	3.070	12.906	45.403	1.00	0.00	H
ATOM	3639	1HB	PRO	346	3.122	10.979	46.298	1.00	0.00	H
ATOM	3640	2HB	PRO	346	1.368	10.826	45.817	1.00	0.00	H
ATOM	3641	1HG	PRO	346	2.149	10.674	48.516	1.00	0.00	H
ATOM	3642	2HG	PRO	346	0.607	11.371	48.025	1.00	0.00	H
ATOM	3643	1HD	PRO	346	1.527	13.382	48.997	1.00	0.00	H
ATOM	3644	2HD	PRO	346	3.240	12.875	48.608	1.00	0.00	H
ATOM	3645	N	ALA	347	1.340	12.674	43.647	1.00	0.00	N
ATOM	3646	CA	ALA	347	0.397	12.667	42.568	1.00	0.00	C
ATOM	3647	C	ALA	347	0.458	11.247	42.104	1.00	0.00	C
ATOM	3648	O	ALA	347	1.475	10.809	41.569	1.00	0.00	O
ATOM	3649	CB	ALA	347	0.792	13.567	41.385	1.00	0.00	C
ATOM	3650	H	ALA	347	2.307	12.386	43.441	1.00	0.00	H
ATOM	3651	HA	ALA	347	-0.599	12.946	42.910	1.00	0.00	H
ATOM	3652	1HB	ALA	347	1.743	14.053	41.599	1.00	0.00	H
ATOM	3653	2HB	ALA	347	0.889	12.961	40.483	1.00	0.00	H
ATOM	3654	3HB	ALA	347	0.023	14.324	41.231	1.00	0.00	H
ATOM	3655	N	ASP	348	-0.637	10.488	42.298	1.00	0.00	N
ATOM	3656	CA	ASP	348	-0.598	9.075	42.046	1.00	0.00	C
ATOM	3657	C	ASP	348	-0.710	8.788	40.583	1.00	0.00	C
ATOM	3658	O	ASP	348	-1.773	8.384	40.115	1.00	0.00	O
ATOM	3659	CB	ASP	348	-1.752	8.323	42.738	1.00	0.00	C
ATOM	3660	CG	ASP	348	-1.502	6.825	42.631	1.00	0.00	C
ATOM	3661	OD1	ASP	348	-0.449	6.363	43.146	1.00	0.00	O
ATOM	3662	OD2	ASP	348	-2.357	6.125	42.025	1.00	0.00	O
ATOM	3663	H	ASP	348	-1.509	10.924	42.629	1.00	0.00	H
ATOM	3664	HA	ASP	348	0.336	8.640	42.401	1.00	0.00	H
ATOM	3665	1HB	ASP	348	-2.689	8.579	42.244	1.00	0.00	H
ATOM	3666	2HB	ASP	348	-1.790	8.619	43.786	1.00	0.00	H
ATOM	3667	N	ILE	349	0.387	8.972	39.819	1.00	0.00	N

ATOM	3668	CA	ILE	349	0.351	8.623	38.427	1.00	0.00	C
ATOM	3669	C	ILE	349	1.763	8.377	37.997	1.00	0.00	C
ATOM	3670	O	ILE	349	2.688	9.009	38.502	1.00	0.00	O
ATOM	3671	CB	ILE	349	-0.191	9.705	37.543	1.00	0.00	C
ATOM	3672	CG1	ILE	349	-1.623	10.074	37.963	1.00	0.00	C
ATOM	3673	CG2	ILE	349	-0.089	9.204	36.094	1.00	0.00	C
ATOM	3674	CD1	ILE	349	-2.147	11.354	37.315	1.00	0.00	C
ATOM	3675	H	ILE	349	1.246	9.361	40.232	1.00	0.00	H
ATOM	3676	HA	ILE	349	-0.259	7.724	38.336	1.00	0.00	H
ATOM	3677	HB	ILE	349	0.421	10.592	37.704	1.00	0.00	H
ATOM	3678	1HG1	ILE	349	-1.638	10.216	39.043	1.00	0.00	H
ATOM	3679	2HG1	ILE	349	-2.286	9.258	37.675	1.00	0.00	H
ATOM	3680	1HG2	ILE	349	0.345	8.204	36.084	1.00	0.00	H
ATOM	3681	2HG2	ILE	349	-1.083	9.171	35.649	1.00	0.00	H
ATOM	3682	3HG2	ILE	349	0.543	9.880	35.518	1.00	0.00	H
ATOM	3683	1HD1	ILE	349	-1.381	11.770	36.660	1.00	0.00	H
ATOM	3684	2HD1	ILE	349	-3.039	11.127	36.731	1.00	0.00	H
ATOM	3685	3HD1	ILE	349	-2.395	12.079	38.090	1.00	0.00	H
ATOM	3686	N	LYS	350	1.974	7.444	37.047	1.00	0.00	N
ATOM	3687	CA	LYS	350	3.316	7.189	36.606	1.00	0.00	C
ATOM	3688	C	LYS	350	3.605	8.177	35.522	1.00	0.00	C
ATOM	3689	O	LYS	350	4.019	7.818	34.421	1.00	0.00	O
ATOM	3690	CB	LYS	350	3.474	5.780	36.012	1.00	0.00	C
ATOM	3691	CG	LYS	350	3.185	4.668	37.025	1.00	0.00	C
ATOM	3692	CD	LYS	350	2.949	3.297	36.387	1.00	0.00	C
ATOM	3693	CE	LYS	350	1.581	3.161	35.710	1.00	0.00	C
ATOM	3694	NZ	LYS	350	1.430	1.810	35.120	1.00	0.00	N
ATOM	3695	H	LYS	350	1.183	6.921	36.643	1.00	0.00	H
ATOM	3696	HA	LYS	350	3.961	7.329	37.473	1.00	0.00	H
ATOM	3697	1HB	LYS	350	4.479	5.585	35.638	1.00	0.00	H
ATOM	3698	2HB	LYS	350	2.805	5.595	35.171	1.00	0.00	H
ATOM	3699	1HG	LYS	350	2.299	4.847	37.634	1.00	0.00	H
ATOM	3700	2HG	LYS	350	3.989	4.506	37.742	1.00	0.00	H
ATOM	3701	1HD	LYS	350	2.995	2.470	37.096	1.00	0.00	H
ATOM	3702	2HD	LYS	350	3.673	3.044	35.612	1.00	0.00	H
ATOM	3703	1HE	LYS	350	1.475	3.900	34.916	1.00	0.00	H
ATOM	3704	2HE	LYS	350	0.782	3.314	36.435	1.00	0.00	H
ATOM	3705	1HZ	LYS	350	2.282	1.260	35.297	1.00	0.00	H
ATOM	3706	2HZ	LYS	350	0.621	1.336	35.547	1.00	0.00	H
ATOM	3707	3HZ	LYS	350	1.280	1.893	34.104	1.00	0.00	H
ATOM	3708	N	LEU	351	3.385	9.468	35.824	1.00	0.00	N
ATOM	3709	CA	LEU	351	3.578	10.539	34.888	1.00	0.00	C
ATOM	3710	C	LEU	351	5.033	10.745	34.635	1.00	0.00	C
ATOM	3711	O	LEU	351	5.466	10.904	33.495	1.00	0.00	O
ATOM	3712	CB	LEU	351	3.084	11.884	35.443	1.00	0.00	C
ATOM	3713	CG	LEU	351	1.577	11.957	35.740	1.00	0.00	C
ATOM	3714	CD1	LEU	351	1.199	13.347	36.283	1.00	0.00	C
ATOM	3715	CD2	LEU	351	0.741	11.549	34.514	1.00	0.00	C
ATOM	3716	H	LEU	351	3.061	9.700	36.774	1.00	0.00	H
ATOM	3717	HA	LEU	351	3.087	10.305	33.943	1.00	0.00	H
ATOM	3718	1HB	LEU	351	3.307	12.656	34.706	1.00	0.00	H
ATOM	3719	2HB	LEU	351	3.608	12.076	36.378	1.00	0.00	H
ATOM	3720	HG	LEU	351	1.296	11.210	36.483	1.00	0.00	H
ATOM	3721	1HD1	LEU	351	2.090	13.971	36.335	1.00	0.00	H
ATOM	3722	2HD1	LEU	351	0.469	13.810	35.619	1.00	0.00	H
ATOM	3723	3HD1	LEU	351	0.769	13.243	37.279	1.00	0.00	H
ATOM	3724	1HD2	LEU	351	1.405	11.293	33.689	1.00	0.00	H
ATOM	3725	2HD2	LEU	351	0.124	10.685	34.764	1.00	0.00	H
ATOM	3726	3HD2	LEU	351	0.099	12.379	34.218	1.00	0.00	H
ATOM	3727	N	VAL	352	5.823	10.712	35.724	1.00	0.00	N
ATOM	3728	CA	VAL	352	7.192	11.128	35.687	1.00	0.00	C
ATOM	3729	C	VAL	352	7.951	10.483	34.586	1.00	0.00	C
ATOM	3730	O	VAL	352	8.415	11.166	33.673	1.00	0.00	O
ATOM	3731	CB	VAL	352	7.941	10.828	36.950	1.00	0.00	C
ATOM	3732	CG1	VAL	352	9.422	11.184	36.731	1.00	0.00	C
ATOM	3733	CG2	VAL	352	7.285	11.599	38.106	1.00	0.00	C
ATOM	3734	H	VAL	352	5.429	10.375	36.614	1.00	0.00	H
ATOM	3735	HA	VAL	352	7.296	12.203	35.542	1.00	0.00	H

ATOM	3736	HB	VAL	352	7.830	9.766	37.170	1.00	0.00	H
ATOM	3737	1HG1	VAL	352	9.559	11.563	35.718	1.00	0.00	H
ATOM	3738	2HG1	VAL	352	9.722	11.947	37.448	1.00	0.00	H
ATOM	3739	3HG1	VAL	352	10.034	10.293	36.870	1.00	0.00	H
ATOM	3740	1HG2	VAL	352	6.439	12.172	37.727	1.00	0.00	H
ATOM	3741	2HG2	VAL	352	6.936	10.894	38.861	1.00	0.00	H
ATOM	3742	3HG2	VAL	352	8.013	12.277	38.550	1.00	0.00	H
ATOM	3743	N	LYS	353	8.094	9.151	34.606	1.00	0.00	N
ATOM	3744	CA	LYS	353	9.002	8.687	33.610	1.00	0.00	C
ATOM	3745	C	LYS	353	8.806	7.241	33.319	1.00	0.00	C
ATOM	3746	O	LYS	353	8.176	6.499	34.070	1.00	0.00	O
ATOM	3747	CB	LYS	353	10.454	8.836	34.085	1.00	0.00	C
ATOM	3748	CG	LYS	353	10.710	8.059	35.379	1.00	0.00	C
ATOM	3749	CD	LYS	353	12.154	8.085	35.881	1.00	0.00	C
ATOM	3750	CE	LYS	353	12.405	9.180	36.921	1.00	0.00	C
ATOM	3751	NZ	LYS	353	13.702	8.961	37.600	1.00	0.00	N
ATOM	3752	H	LYS	353	7.603	8.531	35.266	1.00	0.00	H
ATOM	3753	HA	LYS	353	8.877	9.224	32.670	1.00	0.00	H
ATOM	3754	1HB	LYS	353	10.710	9.877	34.280	1.00	0.00	H
ATOM	3755	2HB	LYS	353	11.161	8.465	33.343	1.00	0.00	H
ATOM	3756	1HG	LYS	353	10.445	7.016	35.204	1.00	0.00	H
ATOM	3757	2HG	LYS	353	10.086	8.491	36.161	1.00	0.00	H
ATOM	3758	1HD	LYS	353	12.877	8.260	35.085	1.00	0.00	H
ATOM	3759	2HD	LYS	353	12.456	7.151	36.355	1.00	0.00	H
ATOM	3760	1HE	LYS	353	11.616	9.178	37.673	1.00	0.00	H
ATOM	3761	2HE	LYS	353	12.425	10.160	36.444	1.00	0.00	H
ATOM	3762	1HZ	LYS	353	14.150	8.115	37.219	1.00	0.00	H
ATOM	3763	2HZ	LYS	353	14.314	9.774	37.442	1.00	0.00	H
ATOM	3764	3HZ	LYS	353	13.544	8.840	38.610	1.00	0.00	H
ATOM	3765	N	MET	354	9.354	6.847	32.154	1.00	0.00	N
ATOM	3766	CA	MET	354	9.425	5.496	31.689	1.00	0.00	C
ATOM	3767	C	MET	354	10.824	5.357	31.183	1.00	0.00	C
ATOM	3768	O	MET	354	11.259	6.172	30.372	1.00	0.00	O
ATOM	3769	CB	MET	354	8.512	5.217	30.480	1.00	0.00	C
ATOM	3770	CG	MET	354	8.587	3.776	29.968	1.00	0.00	C
ATOM	3771	SD	MET	354	7.756	2.535	31.007	1.00	0.00	S
ATOM	3772	CE	MET	354	6.075	3.003	30.504	1.00	0.00	C
ATOM	3773	H	MET	354	9.754	7.577	31.548	1.00	0.00	H
ATOM	3774	HA	MET	354	9.207	4.897	32.574	1.00	0.00	H
ATOM	3775	1HB	MET	354	8.734	5.833	29.609	1.00	0.00	H
ATOM	3776	2HB	MET	354	7.453	5.387	30.678	1.00	0.00	H
ATOM	3777	1HG	MET	354	9.638	3.494	29.905	1.00	0.00	H
ATOM	3778	2HG	MET	354	8.117	3.742	28.985	1.00	0.00	H
ATOM	3779	1HE	MET	354	6.124	3.824	29.788	1.00	0.00	H
ATOM	3780	2HE	MET	354	5.582	2.147	30.041	1.00	0.00	H
ATOM	3781	3HE	MET	354	5.507	3.318	31.379	1.00	0.00	H
ATOM	3782	N	SER	355	11.596	4.352	31.648	1.00	0.00	N
ATOM	3783	CA	SER	355	12.917	4.301	31.093	1.00	0.00	C
ATOM	3784	C	SER	355	13.571	2.984	31.369	1.00	0.00	C
ATOM	3785	O	SER	355	13.150	2.232	32.246	1.00	0.00	O
ATOM	3786	CB	SER	355	13.859	5.371	31.662	1.00	0.00	C
ATOM	3787	OG	SER	355	14.104	5.120	33.038	1.00	0.00	O
ATOM	3788	H	SER	355	11.261	3.674	32.347	1.00	0.00	H
ATOM	3789	HA	SER	355	12.897	4.439	30.012	1.00	0.00	H
ATOM	3790	1HB	SER	355	13.408	6.358	31.557	1.00	0.00	H
ATOM	3791	2HB	SER	355	14.807	5.356	31.125	1.00	0.00	H
ATOM	3792	HG	SER	355	13.991	5.993	33.572	1.00	0.00	H
ATOM	3793	N	TRP	356	14.625	2.669	30.584	1.00	0.00	N
ATOM	3794	CA	TRP	356	15.405	1.496	30.852	1.00	0.00	C
ATOM	3795	C	TRP	356	16.875	1.764	30.729	1.00	0.00	C
ATOM	3796	O	TRP	356	17.302	2.676	30.022	1.00	0.00	O
ATOM	3797	CB	TRP	356	14.971	0.189	30.139	1.00	0.00	C
ATOM	3798	CG	TRP	356	14.288	0.285	28.795	1.00	0.00	C
ATOM	3799	CD1	TRP	356	12.945	0.377	28.575	1.00	0.00	C
ATOM	3800	CD2	TRP	356	14.905	0.228	27.497	1.00	0.00	C
ATOM	3801	NE1	TRP	356	12.682	0.370	27.230	1.00	0.00	N
ATOM	3802	CE2	TRP	356	13.878	0.279	26.553	1.00	0.00	C
ATOM	3803	CE3	TRP	356	16.215	0.128	27.121	1.00	0.00	C

```
ATOM   3804  CZ2 TRP   356      14.143   0.230  25.215  1.00  0.00           C
ATOM   3805  CZ3 TRP   356      16.478   0.094  25.768  1.00  0.00           C
ATOM   3806  CH2 TRP   356      15.463   0.142  24.835  1.00  0.00           C
ATOM   3807  H   TRP   356      14.869   3.275  29.788  1.00  0.00           H
ATOM   3808  HA  TRP   356      15.233   1.116  31.859  1.00  0.00           H
ATOM   3809  HC  TRP   356      17.579   1.138  31.276  1.00  0.00           H
ATOM   3810 1HB  TRP   356      14.267  -0.319  30.798  1.00  0.00           H
ATOM   3811 2HB  TRP   356      15.871  -0.403  29.977  1.00  0.00           H
ATOM   3812  HD1 TRP   356      12.189   0.446  29.357  1.00  0.00           H
ATOM   3813  HE1 TRP   356      11.748   0.423  26.798  1.00  0.00           H
ATOM   3814  HE3 TRP   356      17.016   0.077  27.858  1.00  0.00           H
ATOM   3815  HZ2 TRP   356      13.341   0.259  24.477  1.00  0.00           H
ATOM   3816  HZ3 TRP   356      17.511   0.027  25.427  1.00  0.00           H
ATOM   3817  HH2 TRP   356      15.711   0.109  23.774  1.00  0.00           H
ATOM   3818  MG  MET   357      21.729  10.606  29.309  1.00  0.00           C
TER
```

WE CLAIM

1. A model for a ligand binding domain of a galactosyltransferase.
2. A model as claimed in claim 1 wherein the ligand binding domain is a binding domain for a disphosphate group of a sugar nucleotide donor, a nucleotide of a sugar nucleotide donor, a nitrogeneous heterocyclic base of a sugar nucleotide donor, a sugar of a nucleotide of a sugar nucleotide donor, a selected sugar of a sugar nucleotide donor that is transferred to an acceptor, or an acceptor.
3. A model of a ligand binding domain as claimed in any of the preceding claims wherein the model comprises one or more of the amino acid residues shown in Table 1 or Figure 2, 3, or 4.
4. A model of a ligand binding domain as claimed in claim 1 comprising hydrogen binding partners for the amide hydrogen, carbonyl oxygen in position 4 and the carbonyl oxygen of uracil.
5. A model of a ligand binding domain as claimed in claim 1 that binds the uridine portion of UDP and comprises Phe-134, Tyr-139, Ile-140, Val-136, Arg-194, Arg-202, Lys-209, Asp-173, His-218, and Thr-137.
6. A model of a ligand binding domain as claimed in claim 1 that interacts with a pyrophosphate portion of UDP comprising Asp-225, Val-226, and Asp-227 of a galactosyltransferase.
7. A model or secondary, tertiary and/or quanternary structure of a galactosyltransferase for an α1,3-galactosyltransferase.
8. A model according to any preceding claims wherein the galactosyltransferase is characterized by the atomic contacts of a galactosyltransferase as shown in Table 1.
9. A model as claimed in claim 8 wherein the atomic contacts are defined by the structural coordinates of the atomic contacts as shown in Table 4 or Table 8.
10. A model according to any preceding claims in association with a ligand or substrate.
11. A model according to any preceding claims having the structural coordinates shown in Table 4 or Table 8.
12. A computer readable medium having stored thereon a model according to any preceding claim.
13. A computerized representation of a model according to any of the preceding claims.
14. A method of screening for a ligand capable of binding a ligand binding domain of a galactosyltransferase comprising the use of a model according to any preceding claim.
15. A ligand identified by a method according to claim 14.
16. A ligand according to claim 15 that is capable of associating with one or more atomic contacts of a galactosyltransferase as shown in Table 1.
17. A secondary and three dimensional structure or model of a ligand binding domain of a galactosyltransferase that associates with a diphosphate of a sugar nucleotide donor comprising atomic interactions 9, 10, and 11 of Table 1, each atomic interaction defined therein by an atomic contact on the diphosphate, and an atomic contact on the galactosyltransferase.
18. A ligand binding domain of a galactosyltransferase that associates with uracil characterized by the following three hydrogen bonds: (1) the amide hydrogen of uracil in position 3 and OD1 of Asp-168 of the galactosyltransferase, (2) the carbonyl oxygen of uracil in position 4 and the side chain of Lys-

204 of the galactosyltransferase, and (3) the carbonyl oxygen of uracil in position 2 and the amide hydrogen of the His-213 side chain of the galactosyltransferase.

19. A secondary or three dimensional structure or model of a ligand binding domain of a galactosyltransferase that associates with a heterocyclic amine base of a sugar nucleotide donor comprising atomic interactions 1, 2, 3, and 4 of Table 1, each atomic interaction defined therein by an atomic contact on the heterocyclic amine base, and an atomic contact on the galactosyltransferase.

20. A secondary and three dimensional structure or model of a ligand binding domain of a galactosyltransferase that associates with a ribose of a sugar nucleotide donor comprising atomic interactions 5, 6, 7, and 8 of Table 1, each atomic interaction defined therein by an atomic contact on the sugar, and an atomic contact on the galactosyltransferase.

21. A secondary or three dimensional structure of a ligand binding domain of a galactosyltransferase that associates with UDP comprising atomic interactions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, or 11 of Table 1, each atomic interaction defined therein by an atomic contact on the nucleotide, and an atomic contact on the galactosyltransferase.

22. A secondary and three dimensional structure or model of a ligand binding domain of a galactosyltransferase that associates with UDP-Gal comprising atomic interactions 1 through 11 of Table 1, each atomic interaction defined therein by an atomic contact on the UDP of the UDP-Gal, and an atomic contact on the galactosyltransferase.

23. A method of identifying a modulator of a galactosyltransferase or a ligand binding domain thereof comprising the step of using the structural coordinates of a galactosysltransferase or a ligand binding domain thereof as shown in Table 4 or 8, or a model according to any preceding claim to computationally evaluate a test compound for its ability to associate with the galactosyltransferase or binding domain or binding site thereof.

24. A method for identifying a potential modulator of a galactosyltransferase by determining binding interactions between a test compound and atomic contacts of a ligand binding domain of a galactosyltransferase comprising:

(a) generating the atomic contacts on a computer screen

(b) generating test compounds with their spatial structure on the computer screen;

(c) determining whether the compounds associate or interact with the atomic contacts defining the galactosyltransferase; and

(d) identifying test compounds that are potential modulators by their ability to enter into a selected number of atomic contacts.

25. A method for identifying a potential modulator of a galactosyltransferase function by docking a computer representation of a test compound with a computer representation of a structure of a galactosyltransferase or a ligand binding domain thereof having the amino acid residues of a galactosytransferase or a ligand binding domain thereof as shown in Table 1 or Figures 3, 4, or 5.

26. A method for the design of ligands for galactosyltransferases based on the three dimensional structure of a sugar nucleotide donor or part thereof comprising using the structural coordinates shown in Table 5, 6, or 7.

27. A method as claimed in claim 26 comprising (a) generating a computer representation of a sugar nucleotide donor, or part thereof, defined by the structural coordinates shown in Table 5, 6, or 7; (b) searching for molecules in a data base that are similar to the defined sugar nucleotide donor, or part thereof, using a searching computer program, or replacing portions of the compound with similar chemical structures from a database using a compound building computer program.

28. A method as claimed in claim 27 comprising one or more of the following additional steps:

(a) testing whether a ligand is a modulator of the activity of a galactosyltransferase in cellular assays and animal model assays;

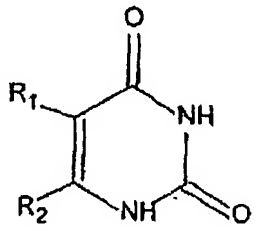
(b) modifying the ligand;

(c) optionally rerunning steps (a) or (b); and

(d) preparing a pharmaceutical composition comprising the modulator.

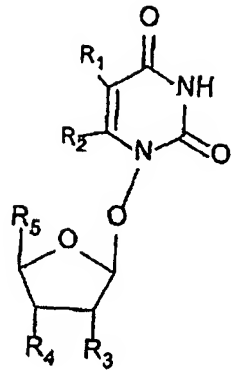
29. A modulator identified by a method of claim 23, 24, 25, or 28.

30. Compounds of the formula I having the structural coordinates of uracil of Table 5, preferably Run 9, Cluster 1 or ATOM 1 to ATOM 9, inclusive of Table 7:



wherein R_1 and R_2 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, pyrophophate, gallic acid, phosphonates, thioamide, and $-OR_{12}$ where R_{12} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring;

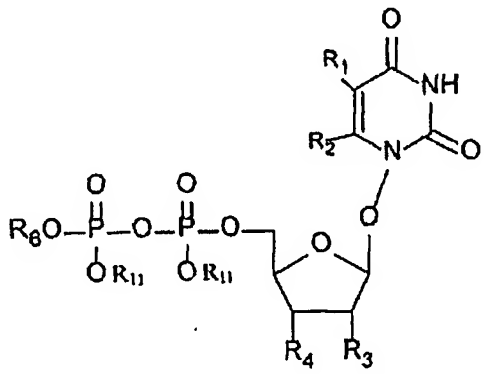
31. Compounds of the following formula II having the structural coordinates of uridine of Table 5, preferably Run 9, Cluster 1 or ATOM 1 to 20 inclusive, of Table 7:



wherein R_1, R_2, R_3, R_4, and R_5 are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof, amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, pyrophosphate, gallic acid, phosphonates, thioamide, and $-OR_{12}$ where R_{12} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring,

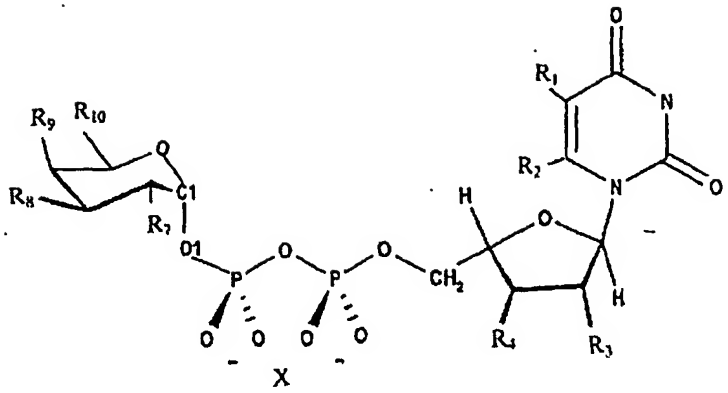
and salts and optically active and racemic forms of a compound of the formula II.

32. Compounds of the formula III having the structural coordinates of UDP in Table 5, preferably Run 9, Cluster 1, or ATOM 1 to 28 inclusive of Table 7:



wherein R_1, R_2, R_3, R_4, R_6, and R_{11} are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol,

33. Compounds of the formula IV having the structural coordinates of UDP-Gal in Table 6, preferably Run, Cluster 1:



wherein R_1, R_2, R_3, R_4, R_7, R_8, R_9, and R_{10} are each independently hydrogen, alkyl, cycloalkyl, alkenyl, alkynyl, heterocyclic rings, aryl, alkoxy, aryloxy, hydroxyl, thiol, thioaryl, amino, halogen, carboxylic acid or esters or thioesters thereof (e.g. $-CH_2OH$), amines, sulfate, sulfonic or sulfinic acid or esters thereof, phosphate, gallic acid, phosphonates, thioamide, and $-OR_{12}$ where R_{12} is alkyl, cycloalkyl, alkenyl, alkynyl, or heterocyclic ring, and X is a counter-ion including sodium, lithium, potassium, calcium, magnesium, manganese, cobalt ions and the like, as well as nontoxic ammonium, quaternary ammonium, and amine cations, preferably Mn^{2+}, and salts and optically active and racemic forms of a compound of the formula IV.

34. A pharmaceutical composition comprising a ligand, modulator, or compound according to any preceding claim, and a pharmaceutically acceptable carrier, diluent, excipient, or adjuvant or any combination thereof.

35. A method of treating and/or preventing disease comprising the step of administering a pharmaceutical composition according to claim 34 to a mammalian patient.

36. A method of treating a disease associated with a galactosyltransferase with inappropriate activity in a cellular organism, comprising:

(a) administering a pharmaceutical composition as claimed in claim 34; and

(b) activating or inhibiting a galactosyltransferase to treat the disease.

37. Use of a modulator or compound as claimed in any of the preceding claims in the preparation of a medicament to treat a disease associated with a galactosyltransferase with inappropriate activity in a cellular organism.

38. Use of the structural coordinates of a galactosyltransferase structure as shown in Table 1 or 8, or the structural coordinates of a ligand as shown in Table 5, 6, or 7 to manufacture a medicament.

39. A computer for producing a model or three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises a galactosyltransferase or ligand binding domain thereof defined by structural coordinates of galactosyltransferase amino acids or a ligand binding domain thereof, or comprises structural coordinates of atoms of a ligand or substrate, or a three-

dimensional representation of a homologue of said molecule or molecular complex, wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine readable data wherein said data comprises the structural coordinates of a galactosyltransferase amino acids according to Table 4 or 8 or a ligand binding domain thereof, or a ligand according to Table 5, 6, or 7;

(b) a working memory for storing instructions for processing said machine-readable data;

(c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

FIGURE 1

```
GALT (     5) gkvilsmlvvstvivvfweyihspegslfwinpsrnpev (43    )
SPSA ( --->  )                                        ( --->  )

GALT (    44) ggssiqkgwwlprwfnngyheedgdineekeqrnedesk (82    )
SPSA ( --->  )                                        ( --->  )

GALT (    83) lklsdwfnpfkrpevvtmtkwkapvvwegtynravldny (121   )
SPSA ( --->  )                                        ( --->  )

GALT (   122) yakqkitvgltvfavgryiehyleefltsankhfmvghp (160   )
SPSA (    A2) P---KVSVIMTSYNKSDYVAKSISSILSQT---F--SDF (A32   )

GALT (   161) vifyimvddvsr--mplielgplrsfkv-fkikpekrwq (196   )
SPSA (   A33) ELF-IMDDNSNEETLNVIRP-FLNDNRVRF---YQS---(  gap )

GALT (   197) dismmrmktigehivahiqhevd-----fl-fcmdvdqv (229   )
SPSA (   A64) DISGVKERTEKTRYAALINQAIEMAEGEYITYATD-DNI (A101  )

GALT (   230) fqdkfgvetlgesvaqlqawwykadpnd-ftyerrkesa (267   )
SPSA (  A102) Y--MP--DRLLKMVRELDT-----HPEKAVIYSASK---(  gap )

GALT (   268) ayipfgeg-dfyyhaaifggtpt-qvlnitqec-----f (299   )
SPSA (  A129) TYHL---N|DIVKETVRPAAQVTWNAPCAIDHCSVMHRY (A166  )

GALT (   300) kgilkdkkndieaqwhdeshlnkyfllnkptkilspeyc (338   )
SPSA ( gap  )-SVLEKVKEKFGSYW-DES-PA-FYRIGD-AR---F-F-(  gap )

GALT (   339) w---dyhiglpadiklvkmswqtkeynvvrnnv       (368   )
SPSA (  A196) WRVNHFYPFYPLDEEL-DLNYIT|EF--VRNLPPQRNCR (A244  )

GALT ( <---  )      -                                ( <---  )
SPSA (  A245) ELRESLKKLGMG                           (A256  )
```

FIGURE 2

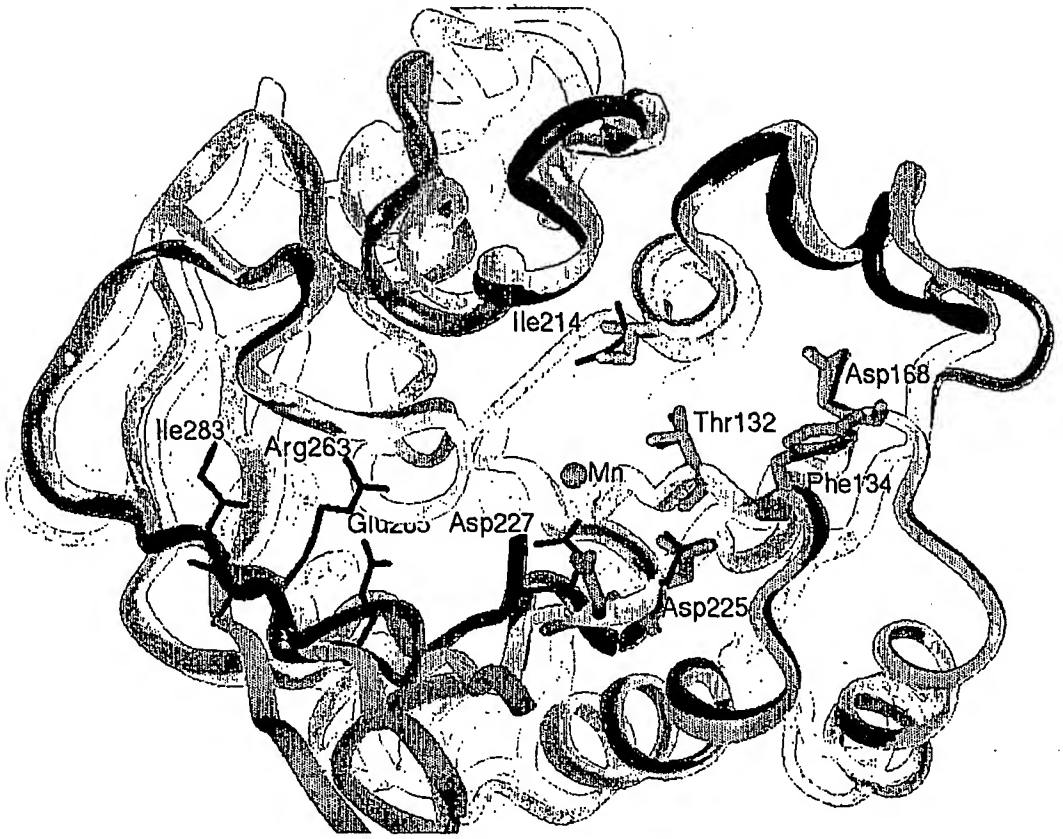

Ile214
Asp168
Thr132
Ile283
Arg263?
Mn
Phe134
Glu265
Asp227
Asp225

FIGURE 3

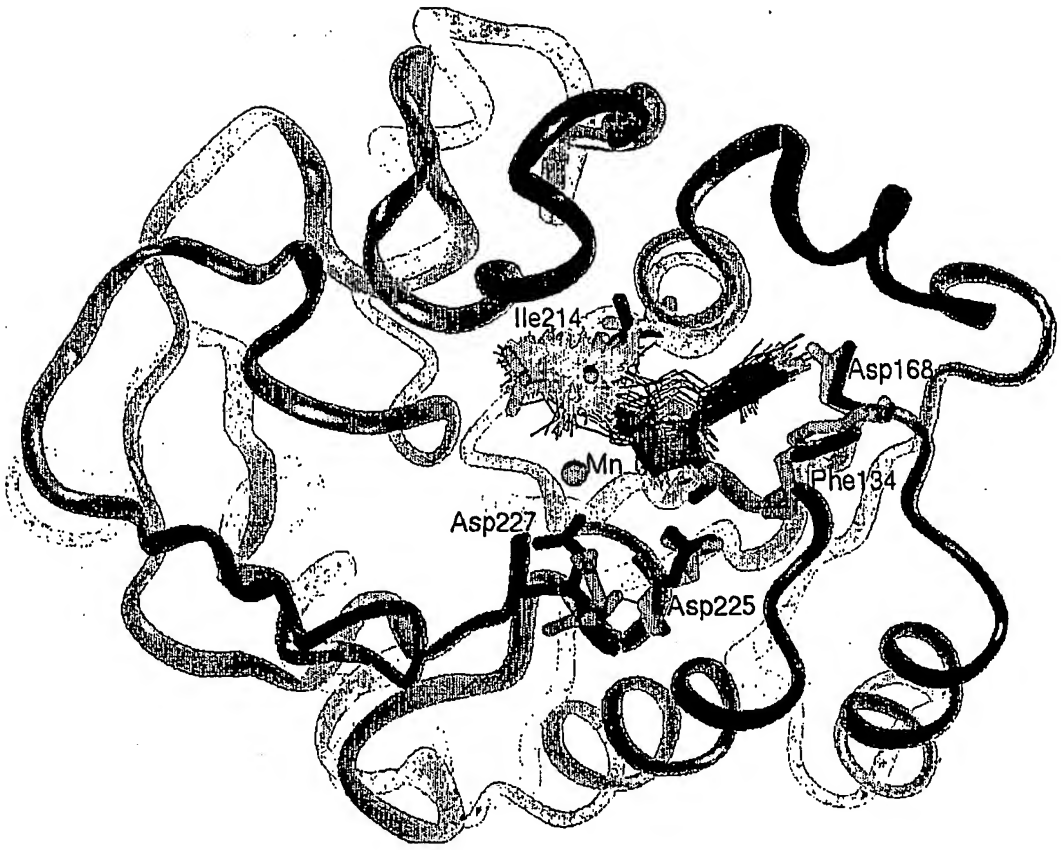


FIGURE 4

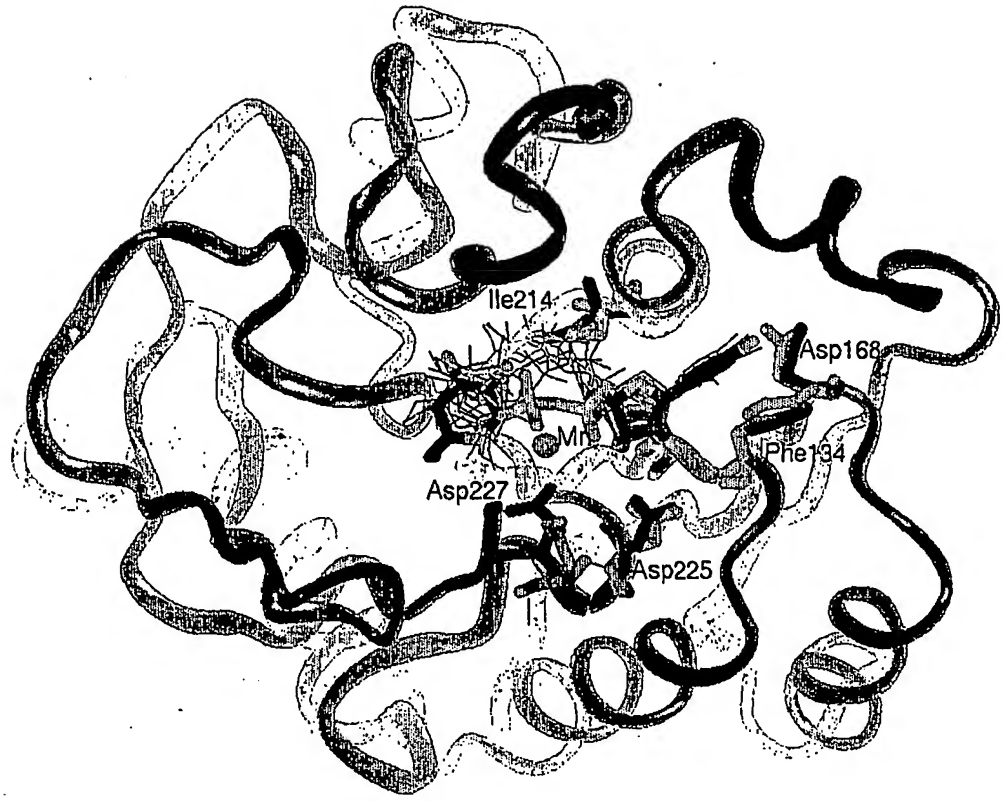


FIGURE 5

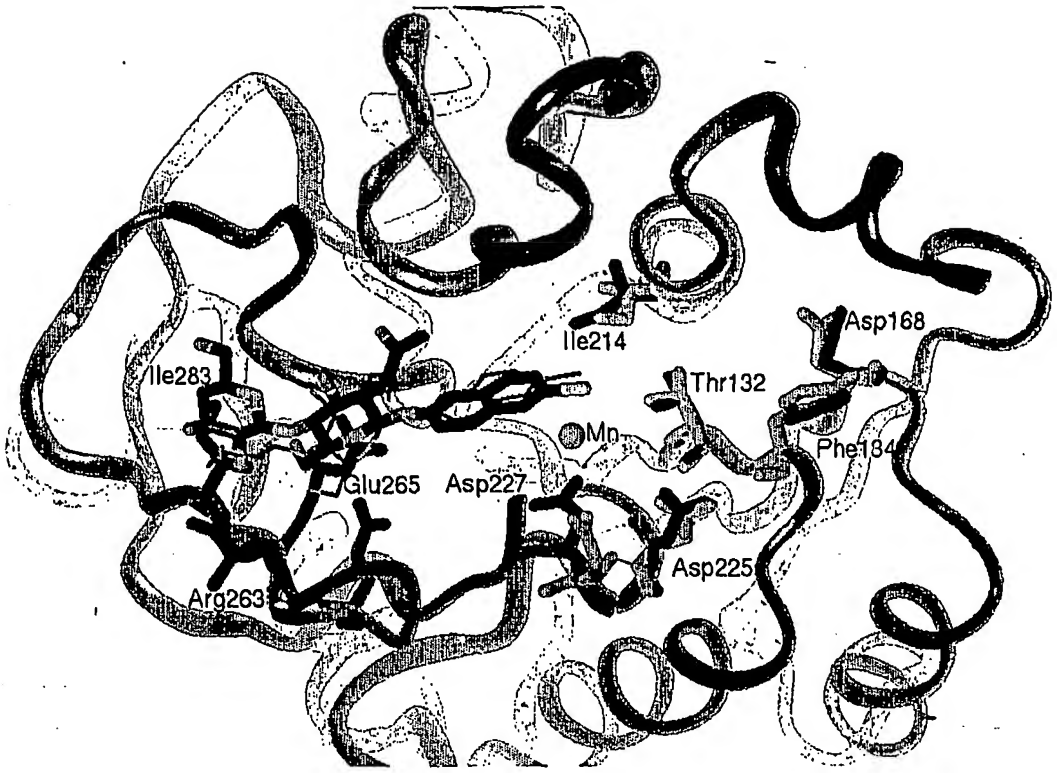

Asp168
Ile214
Ile283
Thr132
Mn
Phe184
Glu265
Asp227
Asp225
Arg263

FIGURE 6

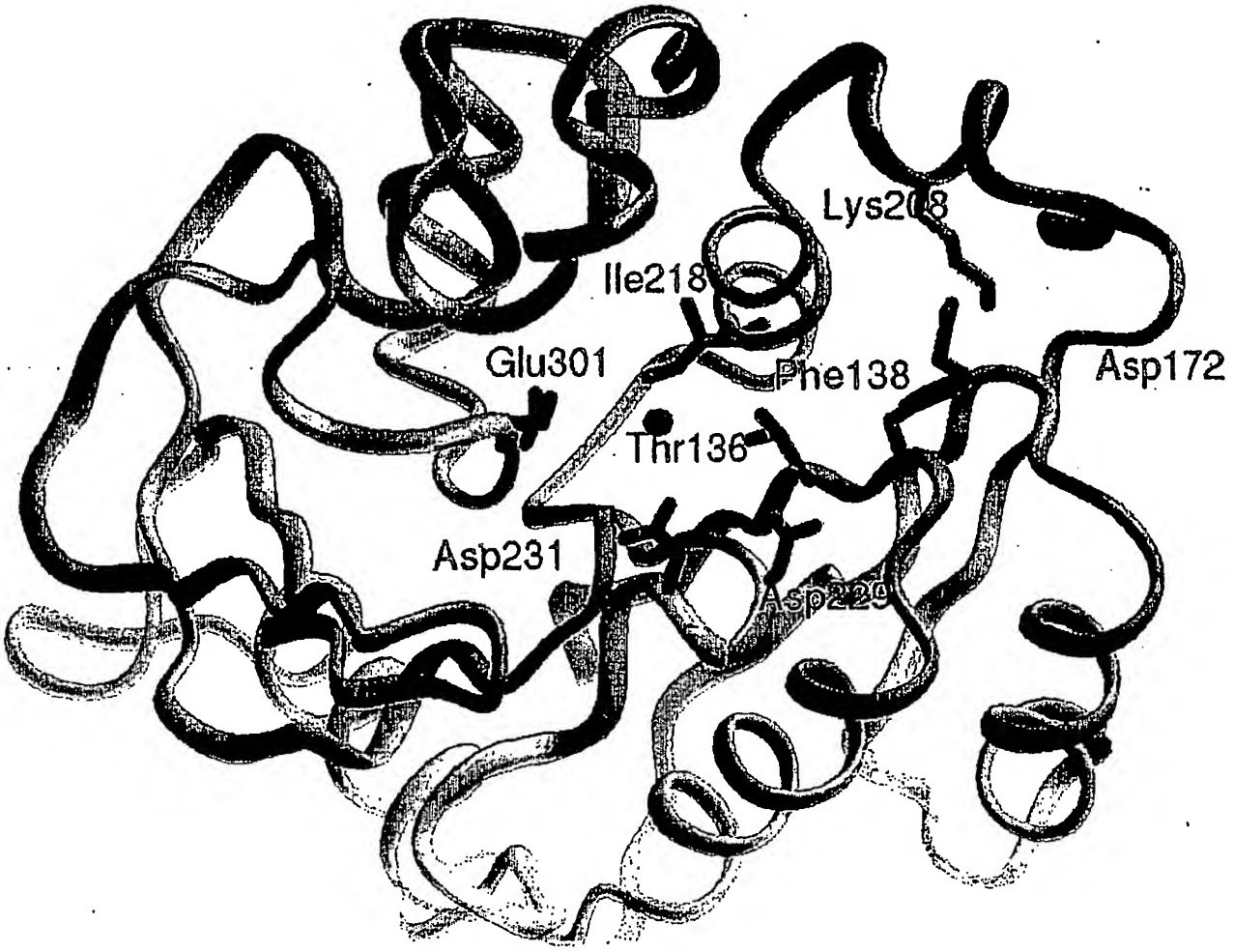


FIGURE 7

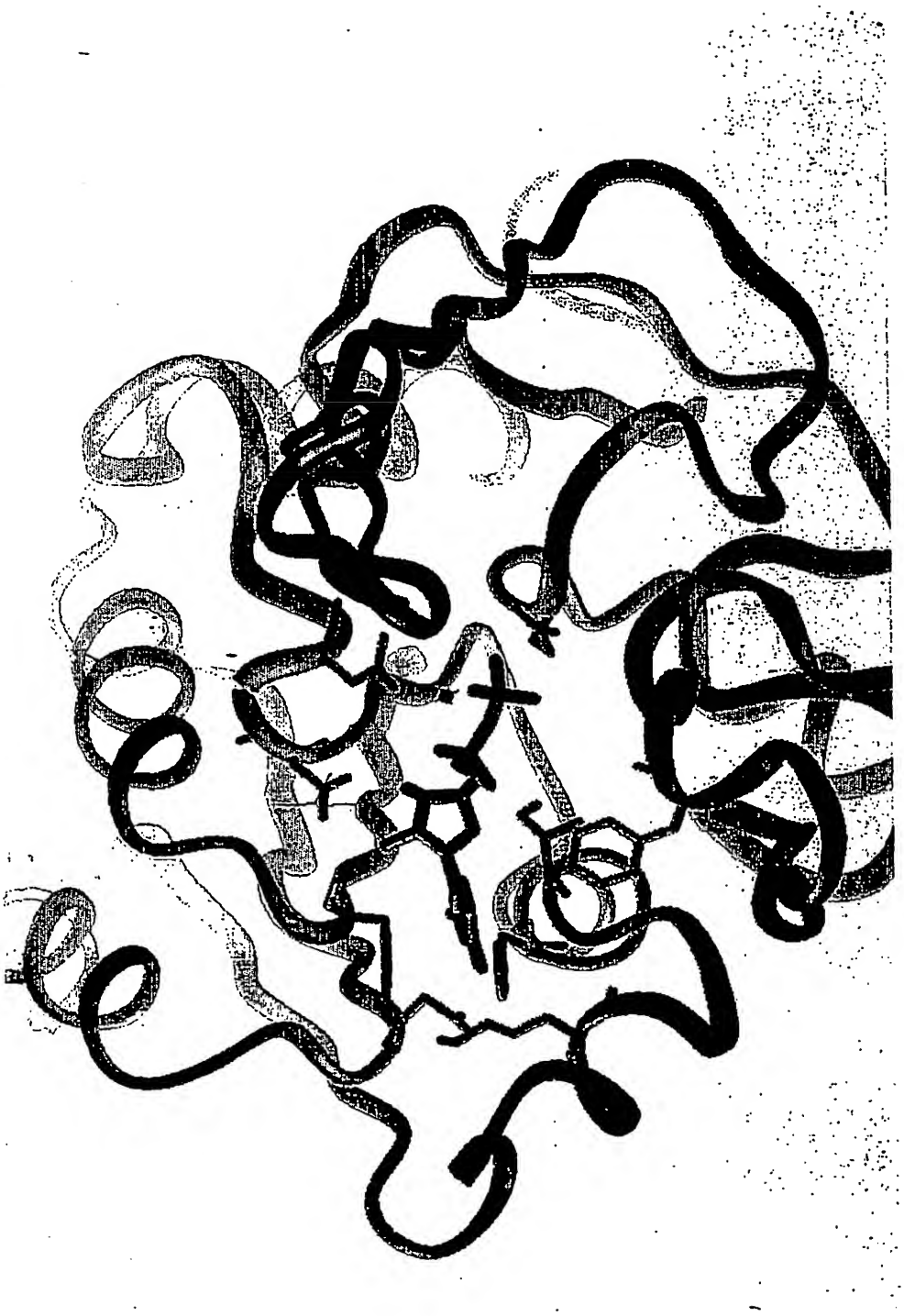
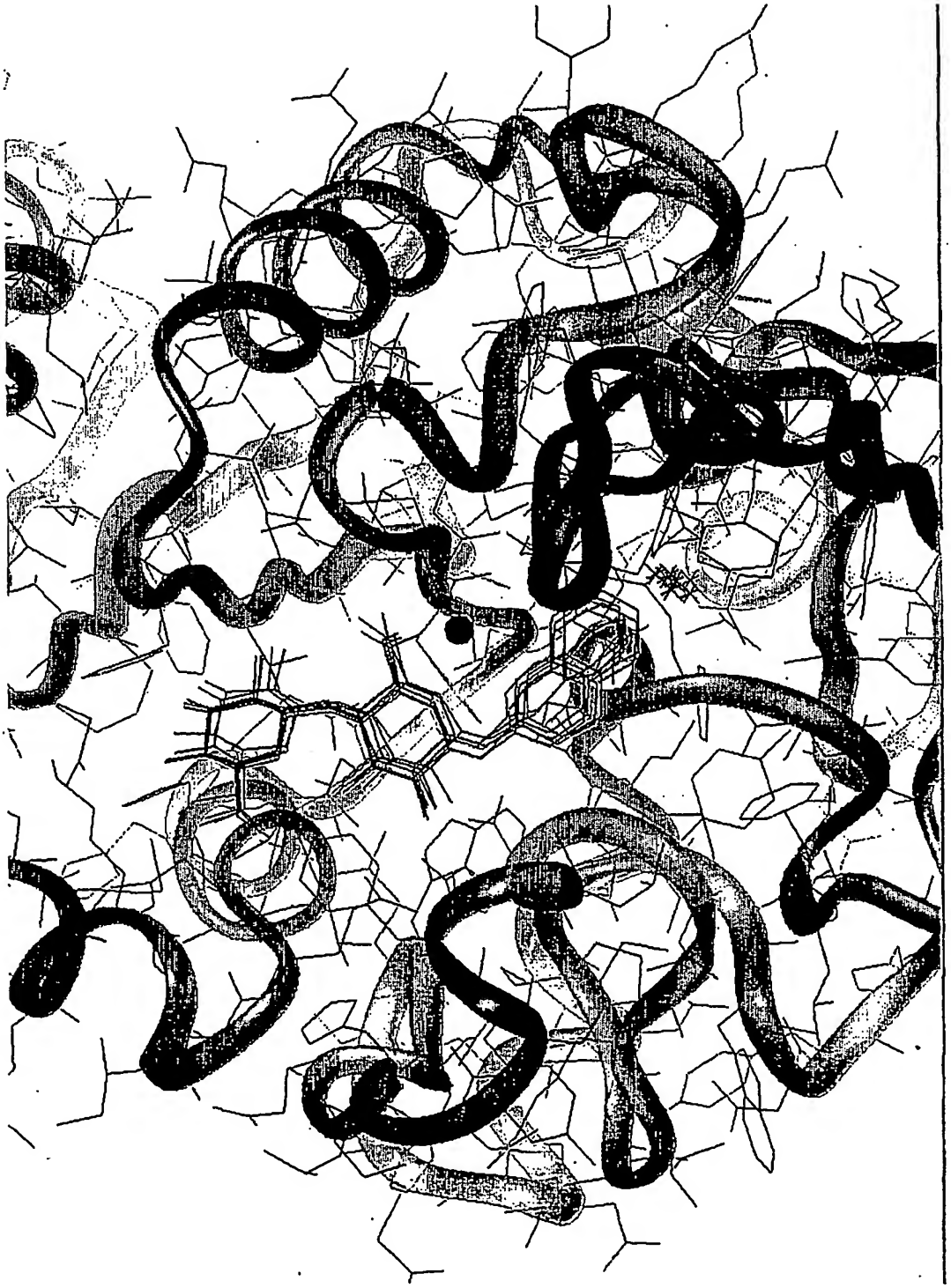


FIGURE 8

FIGURE 9



(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
8 November 2001 (08.11.2001)

PCT

(10) International Publication Number
WO 01/083717 A3

(51) International Patent Classification[7]: C12N 9/10, G06F 19/00, C07D 239/54, C07H 19/073, 19/10, A61K 31/513, 31/7072, C07H 19/06, G06F 17/50

(21) International Application Number: PCT/CA01/00607

(22) International Filing Date: 2 May 2001 (02.05.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/201,841 3 May 2000 (03.05.2000) US

(71) Applicant *(for all designated States except US)*: **GLYCODESIGN INC.** [CA/CA]; 480 University Avenue, Suite 400, Toronto, Ontario M5G 1V2 (CA).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **RAO, Mohan** [IN/CA]; 95 Thorncliffe Park Drive, Apartment 3409, Toronto, Ontario M4H 1L7 (CA). **TVAROSKA, Igor** [SK/CA]; 65 High Park Avenue, Apartment 2201, Toronto, Ontario M6P 2R7 (CA).

(74) Agents: **VAN ZANT, Joan M.** et al.; Swabey Ogilvy Renault, Suite 1600, 1981 McGill College Avenue, Montreal, Québec H3A 2Y3 (CA).

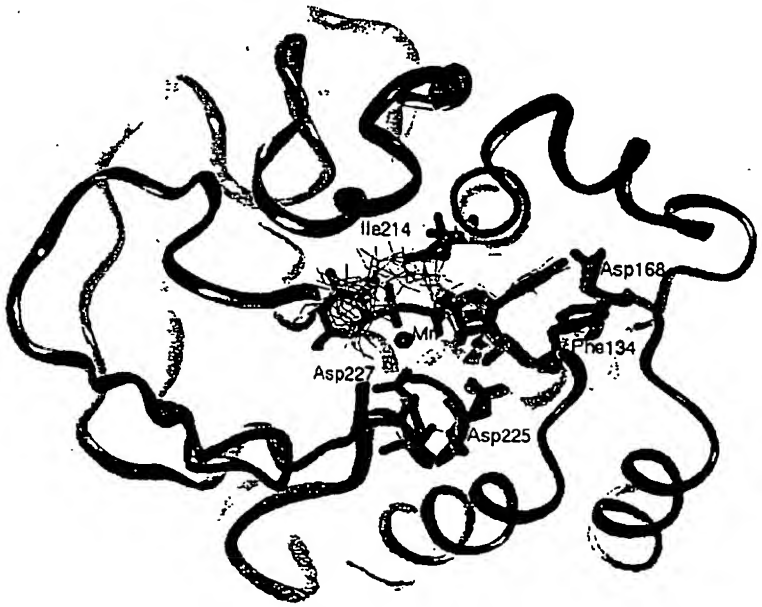
(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW.

(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
— *with international search report*

[Continued on next page]

(54) Title: DESIGNING MODULATORS FOR ALPHA-1, 3 GALACTOSYLTRANSFERASES BASED ON A STRUCTURAL MODEL



(57) Abstract: The invention relates to structures and models of ligand binding domains of galactosyltransferases, and the ligand binding domains with ligands. The structural coordinates that define the structures and any ligands bound to the structures enable the determination of homologues, the structures of polypeptides with unknown structure, and the identification of modulators of the galactosyltransferases. The invention also relates to structures and models of nucleotide-sugar donors for the galactosyltransferases, and the design of modulators for the galactosyltransferases based on the properties of these structures and models.

WO 01/083717 A3

(88) Date of publication of the international search report:
8 August 2002

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

INTERNATIONAL SEARCH REPORT

International Application No
PCT/CA 01/00607

A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C12N9/10 G06F19/00 C07D239/54 C07H19/073 C07H19/10
A61K31/513 A61K31/7072 C07H19/06 G06F17/50

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 C12N G06F G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, BIOSIS, EMBL, CHEM ABS Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	CHARNOCK SIMON J ET AL: "Structure of the nucleotide-diphospho-sugar transferase, SpsA from Bacillus subtilis, in native and nucleotide-complexed forms" BIOCHEMISTRY, AMERICAN CHEMICAL SOCIETY. EASTON, PA, US, vol. 38, no. 20, 18 May 1999 (1999-05-18), pages 6380-6385, XP001038468 ISSN: 0006-2960	18,32
Y	pages 6381-6382 and Figure 4	14,23-28

-/--

[X] Further documents are listed in the continuation of box C.

[X] Patent family members are listed in annex.

* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
30 January 2002	26/02/2002

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Vix, O

Form PCT/ISA/210 (second sheet) (July 1992)

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	IMBERTY ANNE ET AL: "Fold recognition study of alpha3-galactosyltransferase and molecular modeling of the nucleotide sugar-binding domain." GLYCOBIOLOGY, vol. 9, no. 7, July 1999 (1999-07), pages 713-722, XP001026527 ISSN: 0959-6658	18,33
Y	abstract, Fig 1, page 717, Fig. 3 and page 719	14,23-28
Y	JOZIASSE D H ET AL: "BOVINE ALPHA-1-3 GALACTOSYLTRANSFERASE ISOLATION AND CHARACTERIZATION OF A COMPLEMENTARY DNA CLONE IDENTIFICATION OF HOMOLOGOUS SEQUENCES IN HUMAN GENOMIC DNA" JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 264, no. 24, 1989, pages 14290-14297, XP001026521 ISSN: 0021-9258 abstract, fig. 2 and page 14296	18,35,36
Y	DATABASE EMBL 'Online! accession P14769, protein EC 2.4.1.151, 1 April 1990 (1990-04-01) JOZIASSE DH ET AL.: "bovine alpha 1-3 galactosyltransferase gene" XP002186993 the whole document	18
X	DATABASE SIGMA-ALDRICH 'Online! Products for Life Science, "search for UDP" retrieved from HTTP://WWW.SIGMA-ALDRICH.COM XP002186994 Uracil, Uridine 5'-diphosphogalactose, Uridine, etc.. are common products listed in different providers catalog	30-33
X	GASTINEL LOUIS NOEL ET AL: "Crystal structures of the bovine beta4galactosyltransferase catalytic domain and its complex with uridine diphosphogalactose." EMBO (EUROPEAN MOLECULAR BIOLOGY ORGANIZATION) JOURNAL, vol. 18, no. 13, 1 July 1999 (1999-07-01), pages 3546-3557, XP002186991 ISSN: 0261-4189	18,33
Y	page 3548-50, Fig 2, 4 ,5 and page 3554	23-28

-/--

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
Y	ASZODI ANDRAS ET AL: "Protein modeling by multiple sequence threading and distance geometry." PROTEINS, no. SUPPL. 1, 1997, pages 38-42, XP001038475 ISSN: 0887-3585 the whole document	18,23-28
Y	CHUNG S J ET AL: "Acceptor substrate-based selective inhibition of galactosyltransferases" BIOORGANIC & MEDICINAL CHEMISTRY LETTERS, OXFORD, GB, vol. 8, no. 23, 1 December 1998 (1998-12-01), pages 3359-3364, XP004143758 ISSN: 0960-894X Fig 1, table 1, page 3362	23-28, 35,36
Y	BRETON CHRISTELLE ET AL: "Structure/function studies of glycosyltransferases." CURRENT OPINION IN STRUCTURAL BIOLOGY, vol. 9, no. 5, October 1999 (1999-10), pages 563-571, XP001026532 ISSN: 0959-440X page 566 and Fig. 4	18,23
A	US 5 849 991 A (CRAWFORD ROBERT J ET AL) 15 December 1998 (1998-12-15) columns 2,4,6,8	18,23-28
A	THODEN JAMES B ET AL: "Structural analysis of UDP-sugar binding to UDP-galactose 4-epimerase from Escherichia coli." BIOCHEMISTRY, vol. 36, no. 21, 1997, pages 6294-6304, XP001038467 ISSN: 0006-2960 page 2558, Figure 4, 6, 7.	30-33
P,Y	UNLIGIL ULUG M ET AL: "X-ray crystal structure of rabbit N-acetylglucosaminyltransferase I: Catalytic mechanism and a new protein superfamily." EMBO (EUROPEAN MOLECULAR BIOLOGY ORGANIZATION) JOURNAL, vol. 19, no. 20, 16 October 2000 (2000-10-16), pages 5269-5280, XP001026132 ISSN: 0261-4189 pp5270 left column, Fig. 2 and 4.	18

-/--

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication,where appropriate, of the relevant passages	Relevant to claim No.
T	RAO MOHAN ET AL: "Structure of bovine alpha-1,3-galactosyltransferase and its complexes with UDP and UDPGal inferred from molecular modeling." PROTEINS, vol. 44, no. 4, 1 September 2001 (2001-09-01), pages 428-434, XP001038482 ISSN: 0887-3585 the whole document	18,23-28

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 1-13,17,19-22, 29, 34-39

Presentation of information:
The claims 1-13, 17, 19-22, 38-39 relate to, or comprise, a three dimensional homology model for the ligand binding domain of a galactosyltransferase or its production which is considered to be a subject-matter encompassed by Rule 39.1(v) and/or (vi) PCT, being subject-matter which the ISA is not required to search under Art. 17(2)(a)(i) PCT. The above mentioned claims relate to a presentation of information (protein model structure coordinates) identified as a coordinates listings and their possible use -claim 38- (using appropriate molecular modelling software), or information stored on a computer (claim 39 and 13) or computer readable media (claim 12). Thus, said claims will not be searched.

Enzyme "ligand/s" or "modulator/s" and their use:
Present claims 15-16, 29, 34-37 relate to a compound (and its use in pharmaceutical composition or in methods of treatment) defined by reference to a its binding property to a glycosyltransferase (a "ligand" or a "modulator" of alpha 1-3 glycosyltransferase).
The claims cover all products having this characteristic or property, whereas the application provides support within the meaning of Article 6 PCT and/or disclosure within the meaning of Article 5 PCT for NONE such products. In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT).
A meaningful search cannot be established because it is not possible to determine if any of the presently known substances is falling under the terms of these "modulator" product claims. Besides it is noted, that the compounds of claims 15-16 and 29 are not rendered novel just because of the fact that they have been identified by the method of claims 23-28, e.g. such compounds can already exist.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

INTERNATIONAL SEARCH REPORT

International Application No
PCT/CA 01/00607

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
US 5849991 A	15-12-1998	AU 695373 B2	13-08-1998
		BR 9506652 A	02-09-1997
		CA 2181433 A1	03-08-1995
		EP 0755451 A1	29-01-1997
		AU 1544595 A	15-08-1995
		AU 711144 B2	07-10-1999
		AU 7742898 A	01-10-1998
		WO 9520661 A1	03-08-1995
		JP 9508277 T	26-08-1997